Atomic to continuum passage for nanotubes. Part I: a discrete Saint-Venant principle

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Contents

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Abstract

We consider general nanotubes of atoms in $\mathbb{R}^3$ where each atom interacts with all others through a two-body potential. When there are no exterior forces, a particular family of nanotubes is the set of perfect nanotubes at the equilibrium. When exterior forces are applied on the nanotube, we compare the nanotube to nanotubes of the previous family. This quantitative comparison is formulated in our main result as a Saint-Venant principle. This estimate can be derived for a large class of potentials (including Lennard-Jones potential), when the perfect nanotubes at the equilibrium are stable. The approach is designed to be applicable to general nanotubes that can be for instance carbon nanotubes or DNA. In a second paper [22] (part II), we derive from our Saint-Venant principle, a macroscopic mechanical model for general nanotubes.

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1 Introduction

In this paper, we study nanotubes that are collections of atoms in $\mathbb{R}^3$. Those atoms are submitted to two-body interactions with all the other atoms and also to exterior forces. Our model can be seen as simplified description of macromolecules like carbon nanotubes or DNA.

We distinguish a subclass of nanotubes that are perfect and at the equilibrium with no exterior forces. Our main result is a quantitative estimate on the distance between a general nanotube and nanotubes of this subclass, namely a Saint-Venant principle (Theorem 1.9).

In order to present our main result we need first to introduce a few concepts and notations in Subsection 1.1. Our assumptions are presented in Subsection 1.2 and should be probably skipped by the reader in a first reading of the introduction. Our main result is given in Subsection 1.3. We discuss the main new difficulties of our approach in Subsection 1.4, and give a brief review of the literature in Subsection 1.5. The organisation of the paper is given in Subsection 1.6.

1.1 The framework

1.1.1 Description of general nanotubes

Given an integer $K \geq 1$ we define

$$\begin{cases} X = (X_j)_{j\in\mathbb{Z}} & \text{with} \quad X_j = (X_{j,l})_{0\leq l\leq K-1} \quad \text{and} \quad X_{j,l} \in \mathbb{R}^3 \\ f = (f_j)_{j\in\mathbb{Z}} & \text{with} \quad f_j = (f_{j,l})_{0\leq l\leq K-1} \quad \text{and} \quad f_{j,l} = \dfrac{1}{K} f_j^0 \in \mathbb{R}^3, \end{cases}$$

Here X is a nanotube, X_j is the j^{th} cell (see Figure 1) containing K atoms, and $f_{j,l}$ is the force acting on the atom $X_{j,l}$. Our particular expression of $f_{j,l}$, i.e.

$$f_{j,l} = \frac{1}{K} f_j^0, \tag{1.1}$$

means that the total force f_j^0 acting on the j^{th} cell is equidistributed on the atoms of the cell.

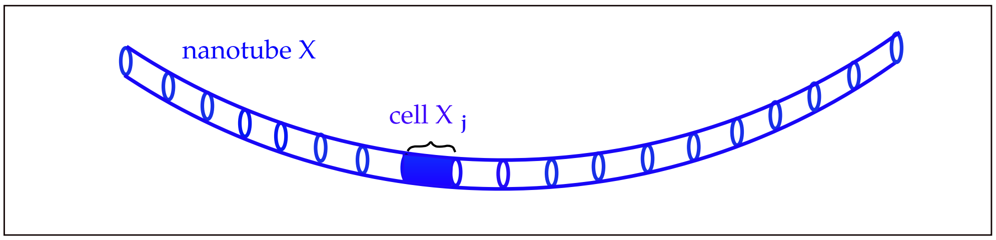

Figure 1: Portion of a nanotube

Given a function $V_0 : (0, \infty) \to \mathbb{R}$, we define the two-body potential as a function of the distance between the atoms:

$$V(L) = V_0(|L|) \quad \text{for every } L \in \mathbb{R}^3 \backslash \{0\}, \tag{1.2}$$

where by convention, we set formally

$$V(0) = 0, \quad \nabla V(0) = 0 \quad \text{and} \quad D^2 V(0) = 0. \tag{1.3}$$

For a general nanotube X we consider the following formal elastic energy as

$$E_0(X) = \frac{1}{2} \sum_{\substack{j, j' \in \mathbb{Z} \\ 0 \leq l, l' \leq K-1}} V(X_{j,l} - X_{j',l'})$$

and the formal total energy as

$$E(X) = E_0(X) + \sum_{\substack{j \in \mathbb{Z} \\ 0 \leq l \leq K-1}} X_{j,l} \cdot f_{j,l}, \tag{1.4}$$

Finally we assume that X solves the corresponding Euler-Lagrange equation

$$E'(X) = 0,$$

i.e.

$$f_{j,l} + \sum_{\substack{j' \in \mathbb{Z} \\ 0 \leq l' \leq K-1}} \nabla V(X_{j,l} - X_{j',l'}) = 0 \quad \text{for any } j \in \mathbb{Z}, \; 0 \leq l \leq K-1. \tag{1.5}$$

Similarly $E_0'(X) = 0$ means (1.5) with $f_{j,l} = 0$.

1.1.2 Perfect nanotubes

Given an angle $\theta \in [0, 2\pi)$ and a vector $L \in \mathbb{R}^3 \backslash \{0\}$, we define the screw displacement $T^{\theta,L}$ by

$$T^{\theta,L}(x) = L + R_{\theta,\widehat{L}}(x) \quad \text{for all } x \in \mathbb{R}^3, \tag{1.6}$$

where $R_{\theta,\widehat{L}}$ is the rotation of angle θ and axis $\widehat{L} = \dfrac{L}{|L|}$.
We define the subclass of **special perfect nanotubes**

$$\mathcal{C}^{\theta,L} = \left\{ X = ((X_{j,l})_l)_j \in ((\mathbb{R}^3)^K)^{\mathbb{Z}},\ X_{j+1,l} = T^{\theta,L}(X_{j,l}) \right\},$$

and the class of **perfect nanotubes**

$$\widehat{\mathcal{C}}^{\theta,L} = \{ Y \in ((\mathbb{R}^3)^K)^{\mathbb{Z}},\ \exists a \in \mathbb{R}^3,\ X \in \mathcal{C}^{\theta,L} \text{ with } Y_{j,l} = a + X_{j,l} \},$$

which is obtained from $\mathcal{C}^{\theta,L}$ by translations.
Examples of perfect nanotubes are represented on Figures 2 and 3.

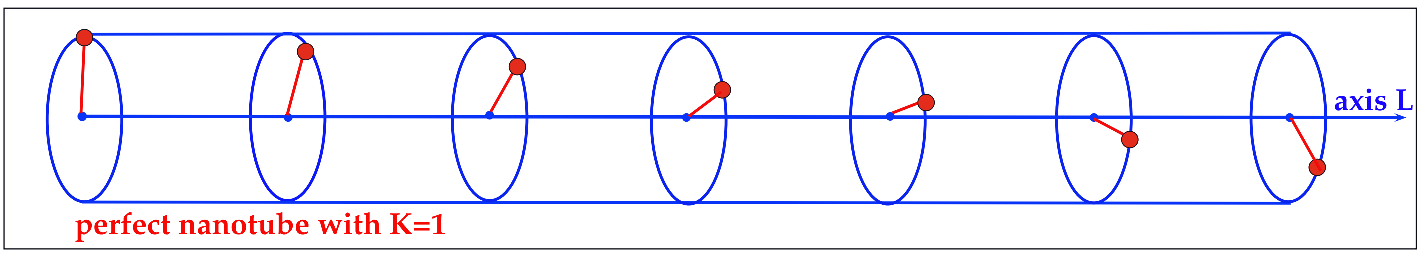

Figure 2: Perfect nanotube with one atom per cell ($K = 1$)

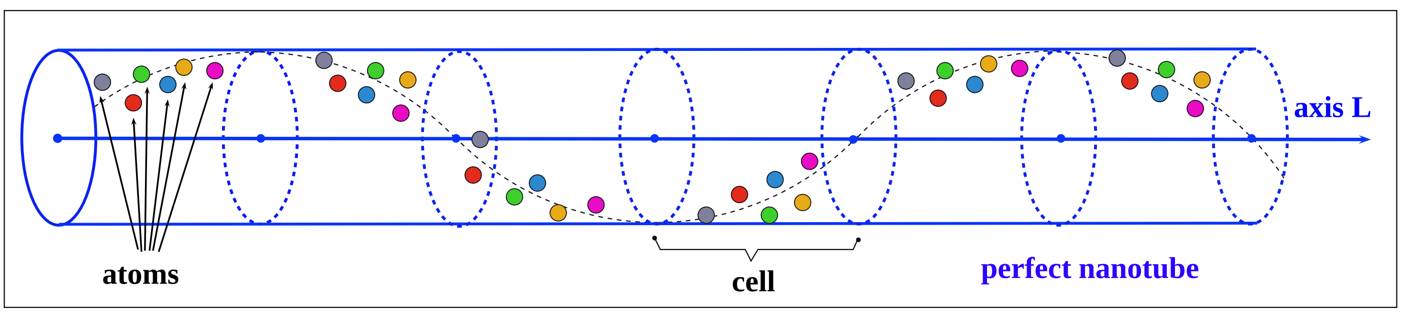

Figure 3: Perfect nanotube with 6 atoms per cell ($K = 6$)

1.1.3 Notation

We will constantly use an abuse of notation writing for any rotation $R \in SO(3)$, $a \in \mathbb{R}^3$ and any cell X_j

$$(R(X_j) + a)_l = R(X_{j,l}) + a.$$

Moreover for a nanotube X we set

$$(R(X)+a)_j = R(X_j)+a.$$

This will be also applied with $\quad R(\cdot) = u \times (\cdot) \quad$ for some $\quad u \in \mathbb{R}^3$.

1.2 Assumptions

In order to state our main results in Subsection 1.3, we need first to introduce several assumptions.

Assumption (H0) (Regularity and decay of the potential)

We assume that $V_0 \in C^2(0,+\infty)$, and for some $p>1$, we assume that

$$\sup_{r\geq 1} r^p \left[|V_0(r)| + r\,|V_0'(r)| + r^2\,|V_0''(r)| \right] < \infty\,.$$

Notice that our assumption (H0) allows us to consider Lennard-Jones potentials. We define the energy per cell of a perfect nanotube $X \in \mathcal{C}^{\theta,L}$ by

$$(1.7)\qquad \begin{aligned} \mathcal{W}(\theta,L,X_0) &= \frac{1}{2} \sum_{\substack{k\,\in\,\mathbb{Z}\\ 0\,\leq\, l,\, m\,\leq\, K-1}} V(X_{k,l}-X_{0,m}) \\ &= \frac{1}{2} \sum_{\substack{k\,\in\,\mathbb{Z}\\ 0\,\leq\, l,\, m\,\leq\, K-1}} V(kL + R_{k\theta,\widehat{L}}(X_{0,l}) - X_{0,m}), \end{aligned}$$

where $X_0 = (X_{0,l})_{0\leq l\leq K-1}$ is a cell for the perfect nanotube X. Notice that $\mathcal{W}$ (up to its second derivatives) is well defined because of assumption (H0) above.

Assumption (H1) (Stability for a particular perfect nanotube)

i) We assume that there exists $\theta^* \in (0, 2\,\pi)$, $L^* \in \mathbb{R}^3\backslash\{0\}$ and $X_0^* = (X_{0,l}^*)_l \in (\mathbb{R}^3)^K$ solution of

$$(1.8)\qquad D_{X_0}\mathcal{W}(\theta^*,L^*,X_0^*) = 0.$$

Let the nanotube $X^* = (X_{j,l}^*) \in \mathcal{C}^{\theta^*,L^*}$ with $X_{j,l}^* = jL^* + R_{j\theta^*,\widehat{L^*}}(X_{0,l}^*)$ for $j \in \mathbb{Z}$ and $0 \leq l \leq K-1$, then we have

$$(1.9)\qquad E_0'(X^*) = 0.$$

We also assume that **not all the atoms $X_{j,l}^*$ are aligned** for $j \in \mathbb{Z}$, $l \in \{0, ..., K-1\}$.
ii) We assume

$$(1.10)\qquad \operatorname{Ker} D^2_{X_0X_0}\mathcal{W}(\theta^*,L^*,X_0^*) = \mathbb{R}(L^* \times X_0^*) + \mathbb{R}\begin{pmatrix} \widehat{L^*} \\ \vdots \\ \widehat{L^*} \end{pmatrix}.$$

where $(L^* \times X_0^*)_l = L^* \times X_{0,l}^*$.

Notice that it is possible to see (see later Proposition 2.3) that (1.8) implies (1.9) in assumption (H1) i).
We will prove later in Proposition 2.4 that under assumption (H1) i) we always have the inclusion

$$\mathbb{R}(L^* \times X_0^*) + \mathbb{R}\begin{pmatrix} \widehat{L^*} \\ \vdots \\ \widehat{L^*} \end{pmatrix} \quad \subset \quad \mathrm{Ker}\, D^2_{X_0X_0}\mathcal{W}(\theta^*, L^*, X_0^*)$$

and therefore (1.10) is a natural assumption of macroscopic stability of the nanotube X^*. Then we have the following result which will be proven later in Subsection 2.2, which provides a parametrisation by (θ, L) of the unit cell $X_0^* = \mathcal{X}_0^*(\theta, L)$ of special perfect nanotubes at the equilibrium.

Proposition 1.1 (Existence of a suitable map $(\theta, L) \mapsto \mathcal{X}_0^*(\theta, L)$)
i) Existence
Assume (H0) and (H1). Then $\mathcal{W}$ is C^2 (on its domain of definition) and there exists a closed neighborhood $\mathcal{U}_0$ of (θ^*, L^*) in $(0, 2\pi) \times (\mathbb{R}^3 \backslash \{0\})$ and a bounded neighborhood $\mathcal{V}_0^*$ of X_0^* in $(\mathbb{R}^3)^K$, and a C^1 map

$$\begin{array}{rccc} \mathcal{X}_0^* & : & \mathcal{U}_0 & \to & \mathcal{V}_0^* \\ & & (\theta, L) & \mapsto & \mathcal{X}_0^*(\theta, L) \end{array}$$

with $\mathcal{X}_0^*(\theta^*, L^*) = X_0^*$, such that for all $(\theta, L) \in \mathcal{U}_0$, we have

$$D_{X_0}\mathcal{W}(\theta, L, \mathcal{X}_0^*(\theta, L)) = 0 \quad \textit{and} \quad \widehat{L} \cdot \left(\sum_{l=0}^{K-1} (\mathcal{X}_0^*)_l(\theta, L) \right) = 0$$

and every $X_0 \in \mathcal{V}_0^*$ solution of

$$D_{X_0}\mathcal{W}(\theta, L, X_0) = 0 \quad \textit{for} \quad (\theta, L) \in \mathcal{U}_0$$

can be writen

$$X_0 = R_{\alpha, \widehat{L}}(\mathcal{X}_0^*(\theta, L)) + \gamma \widehat{L} \quad \textit{for some} \quad \alpha, \gamma \in \mathbb{R}. \tag{1.11}$$

ii) Further technical properties
Up to reduce $\mathcal{U}_0$, we can always show that for any $(\theta, L) \in \mathcal{U}_0$ and

$$\mathcal{X}^*(\theta, L) = (\mathcal{X}_j^*(\theta, L))_{j \in \mathbb{Z}} \quad \textit{with} \quad \mathcal{X}_j^*(\theta, L) = R_{j\theta, \widehat{L}}(\mathcal{X}_0^*(\theta, L)) + jL, \tag{1.12}$$

we have

(1.13) *there are at least three atoms of the nanotube $\mathcal{X}^*(\theta, L)$ which are not aligned,*

$$\mathcal{U}_0 = \overline{Int\, \mathcal{U}_0} \tag{1.14}$$

and there exists $c_0 > 0$ such that

$$\textit{for all} \quad (\theta, L), \ (\bar{\theta}, \bar{L}) \in \mathcal{U}_0, \quad \left\{ \begin{array}{l} |\widehat{L} + \widehat{\bar{L}}| \geq c_0 > 0 \\ |L| - |L - \bar{L}| \geq c_0 > 0, \end{array} \right. \tag{1.15}$$

and (for $r \geq 1$ given such that $r\theta^* \neq 0\,(2\pi)$) we have

$$r\theta \neq 0\,(2\pi) \quad \textit{for all} \quad (\theta, L) \in \mathcal{U}_0. \tag{1.16}$$

Definition 1.2 (The hessian of the energy)
For a nanotube X^*, the hessian of the energy $E_0''(X^*) : ((\mathbb{R}^3)^K)^{\mathbb{Z}} \to ((\mathbb{R}^3)^K)^{\mathbb{Z}}$ is defined for any $Z \in ((\mathbb{R}^3)^K)^{\mathbb{Z}}$ by

$$(E_0''(X^*) \cdot Z)_{j,l} = \sum_{\substack{j' \in \mathbb{Z} \\ 0 \le l' \le K-1}} D^2V(X^*_{j,l} - X^*_{j',l'}) \cdot (Z_{j,l} - Z_{j',l'}).$$

Assumption (H2) (Microscopic stability by characterisation of the kernel of the hessian)

We assume that there exists a positive constant C such that for any $Z \in ((\mathbb{R}^3)^K)^{\mathbb{Z}}$ such that

$$\left\{ \begin{array}{l} E_0''(X^*) \cdot Z = 0 \\ |Z_j| \le C(1 + |j|^2) \end{array} \right. \tag{1.17}$$

then there exist two vectors $u_1, u_2 \in \mathbb{R}^3$ and $(\overline{\theta}, \overline{L}) \in \mathbb{R} \times \mathbb{R}^3$ and $Y \in ((\mathbb{R}^3)^K)^{\mathbb{Z}}$ such that

$$Z = u_1 + u_2 \times X^* + Y, \tag{1.18}$$

with

$$\left\{ \begin{array}{l} X^* = \mathcal{X}^*(\theta^*, L^*) = (\mathcal{X}^*_j(\theta^*, L^*))_{j \in \mathbb{Z}} \quad \text{with} \quad \mathcal{X}^*_j(\theta, L) = R_{j\theta, \widehat{L}}(\mathcal{X}^*_0(\theta, L)) + jL \\ Y = (\bar{\theta}, \bar{L}) \cdot \nabla_{(\theta,L)} \mathcal{X}^*(\theta, L). \end{array} \right.$$

Notice that all Z as in (1.18) are in the kernel of $E''(X^*)$ by Proposition 2.5. Assumption (H2) claims that the kernel defined by (1.17) does not contain other elements. Therefore assumption (H2) appears as a kind of microscopic stability assumption.

Remark 1.3
We can write

$$\left\{ \begin{array}{l} Y_j = \left(R_{j\theta, \widehat{L}}(Y_0) + \overline{\theta} \cdot (j\widehat{L} \times R_{j\theta, \widehat{L}}(X^*_0)) + \overline{L} \cdot \left(\nabla_L R_{j\theta, \widehat{L}}\right)(X^*_0) + j\overline{L} \right) \Big|_{(\theta,L)=(\theta^*,L^*)} \\ \\ Y_0 = (\overline{\theta}, \overline{L}) \cdot \nabla_{(\theta,L)} \mathcal{X}^*_0(\theta, L) \Big|_{(\theta^*,L^*)} \end{array} \right.$$

where we recall that $X^*_0 = \mathcal{X}^*_0(\theta^*, L^*)$.

For later use we introduce the following technical assumption:

Assumption (H3) (Minimal number of cells $2q_0 + 1$ to define the distance D_j)

We introduce conditions on some parameter

$$q_0 = 2r - 1$$

involved later in Definition 1.7, where $2q_0 + 1$ is the minimal number of cells used to define the distance D_j.
If $K \ge 3$ and not all atoms of $\mathcal{X}^*_0(\theta, L)$ are aligned for each $(\theta, L) \in \mathcal{U}_0$, we set

$$r = 1.$$

Otherwise if $K \geq 2$, we set

$$\begin{cases} r = 2 & \text{if} \quad \theta^* \neq \pi \\ r = 3 & \text{if} \quad \theta^* = \pi. \end{cases}$$

If $K = 1$, we set

$$\begin{cases} r = 3 & \text{if} \quad \theta^* \neq \dfrac{2\pi}{3} \quad \text{and} \quad \theta^* \neq \dfrac{4\pi}{3} \\ r = 4 & \text{if} \quad \theta^* = \dfrac{2\pi}{3} \quad \text{or} \quad \theta^* = \dfrac{4\pi}{3}. \end{cases}$$

Remark 1.4
Here $q_0 = 2r - 1$ is such that the atoms of $X_0(\theta, L)$,..., $X_{r-1}(\theta, L)$ are always not all aligned when assumption (H1) i) is satisfied. Moreover $r\theta^* \neq 0\,(2\pi)$, and this condition is used in (1.16).

1.3 Main results

In order to give our main results in Subsection 1.3.2, we first need some definitions in Subsection 1.3.1.

1.3.1 Perfect nanotubes at the equilibrium, distance and semi-norm

A nanotube $X \in \mathcal{C}^{\theta,L}$ is at the equilibrium if $E_0'(X) = 0$. We introduce the following definitions.

Definition 1.5 (Class $C_*^{\theta,L}$)
For any $(\theta, L) \in \mathcal{U}_0$, we define the subclass of perfect nanotubes at the equilibrium by

$$\mathcal{C}_*^{\theta,L} = \{Y \in \mathcal{C}^{\theta,L},\ E_0'(Y) = 0,\ \exists(\alpha,\gamma) \in \mathbb{R}^2,\ Y_0 = R_{\alpha,\widehat{L}}(\mathcal{X}_0^*(\theta, L)) + \gamma \widehat{L}\}.$$

Notice that $\mathcal{X}_0^*(\theta, L)$ is a parametrisation of the unit cell given by Proposition 1.1.

Definition 1.6 (Class $\widehat{C}_*^{\theta,L}$)
For any $(\theta, L) \in \mathcal{U}_0$, we define the class of the perfect nanotubes at the equilibrium by

$$\widehat{\mathcal{C}}_*^{\theta,L} = \{Y \in \widehat{\mathcal{C}}^{\theta,L}, \exists a \in \mathbb{R}^3, X \in \mathcal{C}_*^{\theta,L},\ Y_j = a + X_j\},$$

which is obtained from $\mathcal{C}_*^{\theta,L}$ by translations.

In order to give our main result we need to test the degree of perfection of a nanotube. To this end, we will define a "three cells distance" (when $q = 1$) for a local control of the degree of perfection of a nanotube, and a semi–norm making the local control a global control.

Definition 1.7 (Distance D_j)
For fixed $q \geq q_0 \geq 1$, with q_0 given in (H3), and for any $(\theta, L) \in \mathcal{U}_0$ and a nanotube X we define

$$D_j(X, \theta, L) = \inf_{\widehat{X}^* \in \widehat{\mathcal{C}}_*^{\theta,L}} \sup_{|\alpha| \leq q} |X_{j+\alpha} - \widehat{X}^*_{j+\alpha}|,$$

where $|X_j| = \sup_{0 \leq l \leq K-1} |X_{j,l}|$.

Similarly we define the force $|f_j| = \sup_{0 \leq l \leq K-1} |f_{j,l}|$.

Definition 1.8 (Semi–norm)
We shall say that a subset $J \subset \mathbb{Z}$ of indices is a box, *(i.e. a discrete interval), if and only if it is the intersection of $\mathbb{Z}$ with an interval. For such a box, J, let us define the semi–norm*

$$\mathcal{N}_J(X) := \sup_{j\in J} \inf_{(\theta,L)\in\mathcal{U}_0} D_j(X,\theta,L).$$

Moreover, for a given $\rho > 0$, we set

$$J_\rho := J + Q_\rho,$$

where $Q_\rho := \{e \in \mathbb{Z}, \text{ such that } |e| \leq \rho\}$. We are now ready to state our main result namely the following Saint-Venant principle for discrete nanotubes.

1.3.2 Statements of the main results

With the notation of Subsection 1.3.1, we have:

Theorem 1.9 (A Saint-Venant principle for nanotubes)
Assume (H0), (H1), (H2) and (H3), where we recall that $\theta^* \in (0, 2\pi)$ and $L^* \in \mathbb{R}^3\backslash\{0\}$. Then there exists $\delta_0 > 0$, $\mu \in (0,1)$, C_1, $C_2 > 0$ such that, for every nanotube $X \in ((\mathbb{R}^3)^K)^\mathbb{Z}$ satisfying the Euler–Lagrange equation (1.5) for some $f \in ((\mathbb{R}^3)^K)^\mathbb{Z}$ satisfying (1.1) and

$$\sup_{j\in\mathbb{Z}} D_j(X,\theta^*,L^*) \leq \delta_0, \tag{1.19}$$

we have for any box *$J \subset \mathbb{Z}$*

$$\mathcal{N}_J(X) \ \leq \ \mu\, \mathcal{N}_{J_\rho}(X) + C_1 \sup_{j\in J_\rho} |f_j|, \tag{1.20}$$

with

$$\rho^p = \frac{C_2}{\mathcal{N}_J(X)}, \tag{1.21}$$

where we recall that $p > 1$ is the decay exponent of the two-body potential given in (H0).

Estimate (1.20) when $f = 0$ on J_ρ is illustrated on Figure 4.

This Saint-Venant principle (1.20) has been obtained following the general lines of the previous works [5, 10, 33, 34], but with substantial difficulties that are mentionned in Subsection 1.4. Concerning Saint-Venant's principle and exponential decay estimates, we refer the reader to [27, 36, 41] and to [31, 32, 30] for a center manifolds approach.

Corollary 1.10 (Liouville result for nanotubes)
Assume (H0), (H1), (H2) and (H3), where we recall that $\theta^* \in (0, 2\pi)$ and $L^* \in \mathbb{R}^3\backslash\{0\}$. Then there exists $\delta_0 > 0$ such that for every nanotube $X \in ((\mathbb{R}^3)^K)^\mathbb{Z}$ satisfying the Euler–Lagrange equation (1.5) with $f = 0$ and

$$\sup_{j\in\mathbb{Z}} D_j(X,\theta^*,L^*) \leq \delta_0, \tag{1.22}$$

then there exists $(\theta_0, L_0) \in \mathcal{U}_0$, such that

$$\sup_{j\in\mathbb{Z}} D_j(X,\theta_0,L_0) = 0,$$

and X is a perfect nanotube.

Notice that it could also be interesting to try to derive for nanotubes a boundary layer estimate similar Corollary 2 of [5], (this would require some substantial additional work).

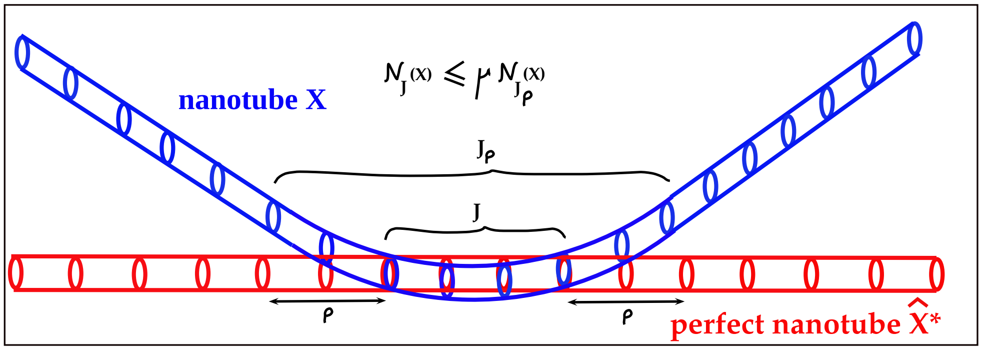

Figure 4: Interpretation of our Saint-Venant principle when $f = 0$ on J_ρ:
X looks more perfect on J than on J_ρ

1.4 Main difficulties encountered

The starting point of our work was paper [5], where a Saint-Venant principle has been obtained for a linear chain of atoms. This Saint-Venant principle was called a Harnack type inequality in [5]. Our goal was to adapt the method to the case of nanotubes in $\mathbb{R}^3$, covering applications for instance to carbon nanotubes and to DNA molecules (in the regime where the bending is neglectable, which is for instance expected when a huge traction is applied). We simplified the analysis, concentrating on the problem with two-body interactions in the case where all the atoms are the same. Nevertheless, we had to face some questions that are several order of magnitude more difficult than in [5]. Even if some proofs may seem elementar from line to line, we had to design from scratch the whole strategy and structure of proof of this paper. For this reason, this paper is fully self-contained. We list below some of the main difficulties encountered here:

1) the definition of perfect nanotubes:

At a first glance a perfect nanotube should be a set of atoms that is invariant by a screw displacement $T^{\theta,L}$ (composition of a rotation $R_{\theta,\widehat{L}}$ and a translation in the direction of the axis L of the rotation). Even if it is very intuitive that we should define a cell repeated by screw displacement, we had to realize that the barycenter of the cell is not necessarily on the axis of the rotation, and then has in general to rotate around this axis. Moreover the parametrisation by $(\theta, L) \in \mathcal{U}_0$ of the family of perfect nanotubes at the equilibrium was not very intuitive, even if it was realised already in [15] that the shape of the microscopic cell of a nanotube can change under homogeneous macroscopic deformations. Moreover, we realised that we had to exclude the case of rotation angle $\theta = 0$ (modulo 2π), which is more singular for at least two reasons: on the one hand several nanotubes families could bifurcate from the case $\theta = 0$ because the dimension of the kernel of $D^2_{X_0X_0}\mathcal{W}$ is higher when $\theta = 0$, and on the other hand the axis of the identity rotation is not well defined. In the same spirit, the suitable stability condition (H2) that we assume on the kernel of the hessian of the microscopic energy was not obvious a priori.

2) the notion of curvature to use:

The statement of our Saint-Venant principle (Theorem 1.9) uses a notion of measure of the degree of imperfection of a general nanotube, which we can interprete as a generalised curvature of the nanotube. When each cell X_k reduces to a single atom and $\theta = 0$ (as in [5]), we can simply consider $D_j(X) := |(X_{k+1} - X_k) - (X_k - X_{k-1})|$ which measures the curvature of the chain of atoms. At the beginning of our work, it was not clear what should be the right corresponding notion $D_j(X, \theta, L)$ for nanotubes and how to use it.

3) rigidity estimates on nanotubes:
Contrarily to the chain of atoms, we have to consider the action of rotations of the nanotube around its axis. This creates a lot of difficulties to estimate the long range position of a general nanotube, from its local generalised curvature $\inf_{(\theta,L)\in\mathcal{U}_0} D_j(X, \theta, L)$.

1.5 Brief review of the literature

Related to our problem is the question of the structure of minimizers of the microscopic problem. In certain cases, periodic minimizers are expected (see for instance the overview [37] and the recent works [18, 4]). Notice that in our problem, perfect nanotubes are not periodic at all, but are only invariant by a screw displacement $T^{\theta,L}$.

Our Saint-Venant principle (1.20) is a kind of quantitative version of the so called Cauchy-Born rule (see [23]), and uses a perturbation argument that shares some similarities with the work [38] on the regularity of solutions of fully non linear elliptic PDEs, or the basic elliptic estimate in [35]. Cases where such Cauchy-Born rule fails (by fracture or melting) have been studied in [6, 13, 42, 26, 16, 24, 12, 11] and a general representation of the macroscopic energy has been given in [1, 14] and in [39, 28, 29] for films. General schemes have been proposed to deduce (assuming the Cauchy-Born rule) macroscopic theories from microscopic ones, see [25, 7, 43, 3]. See also [2, 8] for stochastic lattices. Even if it is different, our approach shares some common points with the Quasi-Continuum Method (see [40]) and some general aspects of multiscale modeling (see the overviews [17, 9]).

A derivation of the Cauchy-Born rule has been obtained in [19] for three-dimensional elasticity starting from microscopic minimizers with two-body interactions of finite range. In [19], the authors use a stability assumption on the Fourier transform of the hessian of the energy, which shares some similarities with our microscopic stability assumption (H2) for nanotubes. Notice that in our present work we do not consider minimizers, but only critical points of the microscopic energy. Extension of [19] to the case of the dynamics is presented in [20].

1.6 Organisation of the paper

This paper is divided into six sections. Section 2 presents certain properties about the equilibrium and the construction (proof of Proposition 1.1) of perfect nanotubes and other properties of the kernel of the hessian of the energy. In Section 3, we prove rough rigidity estimates which are various local and global comparison estimates between nanotubes. In Section 4, we present a fine rigidity estimate (Theorem 4.1) which plays a crucial role in our analysis. This fine estimate compares a general nanotube to a perfect nanotube. In Section 5, we prove our main result (Theorem 1.9), namely a Saint-Venant principle on nanotubes. Finally Section 6 is an appendix, which contains some fundamental results about control of rotations and an axiomatic approach to the definition of perfect nanotubes.

2 Properties of perfect nanotubes

This section is divided in three subsections. In Subsection 2.1 we mainly prove Proposition 2.3 for the equilibrium of perfect nanotubes. In Subsection 2.2 we show Proposition 1.1 and Proposition 2.4 for the construction of a family of perfect nanotubes at the equilibrium. Finaly in Subsection 2.3 we get Proposition 2.5 on the properties of the kernel of the hessian of the energy.

2.1 The equilibrium of perfect nanotubes

In this subsection, we grasp a few results that will be used later in the paper. We first notice that using (H0) we can estimate the rest of the series defining $\mathcal{W}$, $D\mathcal{W}$ and $D^2\mathcal{W}$, and then show that $\mathcal{W} \in C^2$, while there are no pairs of atoms in X that touch each other.

Lemma 2.1 (Computation of $D_{X_{0,l}}\mathcal{W}(\theta, L, X_0)$)
Let us consider a nanotube $X \in \mathcal{C}^{\theta,L}$, then for the energy per cell defined in (1.7) we have

$$D_{X_{0,l}}\mathcal{W}(\theta, L, X_0) = \sum_{\substack{j' \in \mathbb{Z} \\ 0 \le l' \le K-1}} \nabla V(X_{0,l} - X_{j',l'})$$

Proof of Lemma 2.1
We have $\quad \mathcal{W}(\theta, L, X_0) = \dfrac{1}{2} \displaystyle\sum_{\substack{j' \in \mathbb{Z} \\ 0 \le l,l' \le K-1}} V(X_{0,l} - j'L - R_{j'\theta,\widehat{L}}(X_{0,l'}))$.

Then

$$\begin{aligned}
D_{X_{0,p}}\mathcal{W}(\theta, L, X_0) &= \frac{1}{2} \sum_{\substack{j' \in \mathbb{Z} \\ 0 \le l,l' \le K-1}} \delta_{lp} \nabla V(X_{0,l} - j'L - R_{j'\theta,\widehat{L}}(X_{0,l'})) \\
&\quad - \frac{1}{2} \sum_{\substack{j' \in \mathbb{Z} \\ 0 \le l,l' \le K-1}} \delta_{l'p} R_{-j'\theta,\widehat{L}} \nabla V(X_{0,l} - j'L - R_{j'\theta,\widehat{L}}(X_{0,l'})) \\
&= \frac{1}{2} \sum_{\substack{j' \in \mathbb{Z} \\ 0 \le l' \le K-1}} \nabla V(X_{0,p} - j'L - R_{j'\theta,\widehat{L}}(X_{0,l'})) \\
&\quad - \frac{1}{2} \sum_{\substack{j' \in \mathbb{Z} \\ 0 \le l \le K-1}} R_{-j'\theta,\widehat{L}} \nabla V(X_{0,l} - j'L - R_{j'\theta,\widehat{L}}(X_{0,p})).
\end{aligned}$$

Using Lemma 6.1 in the appendix, we compute

$$\begin{aligned}
& -\frac{1}{2} \sum_{\substack{j' \in \mathbb{Z} \\ 0 \le l \le K-1}} R_{-j'\theta,\widehat{L}} \nabla V(X_{0,l} - j'L - R_{j'\theta,\widehat{L}}(X_{0,p})) \\
= & -\frac{1}{2} \sum_{\substack{j' \in \mathbb{Z} \\ 0 \le l \le K-1}} \nabla V\Big(R_{-j'\theta,\widehat{L}}\big(X_{0,l} - j'L - R_{j'\theta,\widehat{L}}(X_{0,p})\big)\Big) \\
= & -\frac{1}{2} \sum_{\substack{j' \in \mathbb{Z} \\ 0 \le l' \le K-1}} \nabla V\big(R_{-j'\theta,\widehat{L}}(X_{0,l'}) - j'L - X_{0,p}\big) \\
= & \ \frac{1}{2} \sum_{\substack{j' \in \mathbb{Z} \\ 0 \le l' \le K-1}} \nabla V\big(X_{0,p} - (-j'L) - R_{-j'\theta,\widehat{L}}(X_{0,l'})\big) \\
= & \ \frac{1}{2} \sum_{\substack{j' \in \mathbb{Z} \\ 0 \le l' \le K-1}} \nabla V\big(X_{0,p} - j'L - R_{j'\theta,\widehat{L}}(X_{0,l'})\big)
\end{aligned}$$

then we have

$$D_{X_{0,p}} \mathcal{W}(\theta, L, X_0) = \sum_{\substack{j' \in \mathbb{Z} \\ 0 \le l' \le K-1}} \nabla V\big(X_{0,p} - j'L - R_{j'\theta,\widehat{L}}(X_{0,l'})\big)$$

and finally

$$D_{X_{0,l}} \mathcal{W}(\theta, L, X_0) = \sum_{\substack{j' \in \mathbb{Z} \\ 0 \le l' \le K-1}} \nabla V(X_{0,l} - X_{j',l'})$$

□

Lemma 2.2 (Rotation of the external forces)
If $X \in \mathcal{C}^{\theta,L}$ solves (1.5), then we have

$$f_{j+1} = R_{\theta,\widehat{L}}(f_j)$$

and

$$\widehat{L} \cdot \sum_{l=0}^{K-1} f_{j,l} = 0 \quad \textit{for all} \quad j \in \mathbb{Z}. \tag{2.1}$$

Proof of Lemma 2.2
Step 1: Proof of $f_{j+1} = R_{\theta,\widehat{L}}(f_j)$
We recall (1.5) for any $j \in \mathbb{Z}$ and $0 \le l \le K-1$

$$f_{j,l} + A_{j,l} = 0 \quad \text{with} \quad A_{j,l} = \sum_{\substack{j' \in \mathbb{Z} \\ 0 \le l' \le K-1}} \nabla V(X_{j,l} - X_{j',l'}) \tag{2.2}$$

Now we compute

$$\begin{aligned}
A_{j+1,l} &= \sum_{\substack{j' \in \mathbb{Z} \\ 0 \le l' \le K-1}} \nabla V(X_{j+1,l} - X_{j'+1,l'}) \\
&= \sum_{\substack{j' \in \mathbb{Z} \\ 0 \le l' \le K-1}} \nabla V(L + R_{\theta,\widehat{L}}(X_{j,l}) - L - R_{\theta,\widehat{L}}(X_{j',l'}))) \\
&= \sum_{\substack{j' \in \mathbb{Z} \\ 0 \le l' \le K-1}} \nabla V(R_{\theta,\widehat{L}}(X_{j,l} - X_{j',l'})) \\
&= R_{\theta,\widehat{L}}\Big(\sum_{\substack{j' \in \mathbb{Z} \\ 0 \le l' \le K-1}} \nabla V(X_{j,l} - X_{j',l'})\Big) \\
&= R_{\theta,\widehat{L}}(A_{j,l}),
\end{aligned}$$

where we have used Lemma 6.1 in the fourth line. From (2.2), we deduce that

$$f_{j+1,l} = R_{\theta,\widehat{L}}(f_{j,l}).$$

Step 2: Proof of $\widehat{L} \cdot \sum_{l=0}^{K-1} f_{j,l} = 0$

Using (2.2), we get

$$\widehat{L} \cdot \sum_{l=0}^{K-1} f_{j,l} + \widehat{L} \cdot \sum_{l=0}^{K-1} A_{j,l} = 0. \tag{2.3}$$

We compute

$$\begin{aligned}
\widehat{L} \cdot \sum_{l=0}^{K-1} A_{j,l} &= \widehat{L} \cdot \sum_{\substack{j' \in \mathbb{Z} \\ 0 \le l,l' \le K-1}} \nabla V((j-j')L + R_{j\theta,\widehat{L}}(X_{0,l}) - R_{j'\theta,\widehat{L}}(X_{0,l'})) \\
&= \sum_{\substack{j' \in \mathbb{Z} \\ 0 \le l,l' \le K-1}} \widehat{L} \cdot \nabla V\big(R_{j\theta,\widehat{L}}\big((j-j')L + X_{0,l} - R_{(j'-j)\theta,\widehat{L}}(X_{0,l'})\big)\big) \\
&= \sum_{\substack{j' \in \mathbb{Z} \\ 0 \le l,l' \le K-1}} R_{-j\theta,\widehat{L}}(\widehat{L}) \cdot \nabla V((j-j')L + X_{0,l} - R_{(j'-j)\theta,\widehat{L}}(X_{0,l'}))
\end{aligned}$$

where we have used Lemma 6.1 in the last line. This shows that

$$\widehat{L} \cdot \sum_{l=0}^{K-1} A_{j,l} = \sum_{\substack{k \in \mathbb{Z} \\ 0 \le l,l' \le K-1}} \widehat{L} \cdot \nabla V(kL + X_{0,l} - R_{-k\theta,\widehat{L}}(X_{0,l'})),$$

Using similar arguments, we get

$$\begin{array}{rcl}\widehat{L}\cdot\displaystyle\sum_{l=0}^{K-1}A_{j,l} &=& \displaystyle\sum_{\substack{k\in\mathbb{Z}\\0\le l,l'\le K-1}}\widehat{L}\cdot\nabla V(-kL+X_{0,l}-R_{k\theta,\widehat{L}}(X_{0,l'}))\\ &=& \displaystyle\sum_{\substack{k\in\mathbb{Z}\\0\le l,l'\le K-1}}\widehat{L}\cdot\nabla V(R_{k\theta,\widehat{L}}(-kL+R_{-k\theta,\widehat{L}}(X_{0,l})-X_{0,l'}))\\ &=& \displaystyle\sum_{\substack{k\in\mathbb{Z}\\0\le l,l'\le K-1}}R_{-k\theta,\widehat{L}}(\widehat{L})\cdot\nabla V(-kL+R_{-k\theta,\widehat{L}}(X_{0,l'})-X_{0,l})\\ &=& \displaystyle\sum_{\substack{k\in\mathbb{Z}\\0\le l,l'\le K-1}}\widehat{L}\cdot\nabla V(kL+R_{k\theta,\widehat{L}}(X_{0,l'})-X_{0,l})\\ &=& -\widehat{L}\cdot\displaystyle\sum_{l=0}^{K-1}A_{j,l},\end{array}$$

This implies that $\widehat{L}\cdot\sum_{l=0}^{K-1}A_{j,l}=0$, which with (2.3) implies (2.1).

$\square$

Finally we have

Proposition 2.3 (Euler-Lagrange equations deriving from $\mathcal{W}$ and E)
Given a solution $X\in\mathcal{C}^{\theta,L}$ of Euler-Lagrange equation (1.5), we have

$$-D_{X_{0,p}}\mathcal{W}(\theta,L,X)=f_{0,p}. \tag{2.4}$$

and

$$D_{X_{0,p}}\mathcal{W}(\theta,L,X)=0 \quad\Longleftrightarrow\quad E_0'(X)=0$$

Proof of Proposition 2.3
By Lemma 2.1, we have

$$D_{X_{0,l}}\mathcal{W}(\theta,L,X_0)=\sum_{\substack{j'\in\mathbb{Z}\\0\le l'\le K-1}}\nabla V(X_{0,l}-X_{j',l'}).$$

Using (1.5), we obtain

$$-D_{X_{0,p}}\mathcal{W}(\theta,L,X_0)=f_{0,p}.$$

If $E_0'(X)=0$, then $f_0=0$ and finally

$$D_{X_{0,p}}\mathcal{W}(\theta,L,X_0)=0.$$

Reciprocically, let us assume that $f_0=0$. Then by Lemma 2.2 we have $f_{j+1}=R_{\theta,\widehat{L}}(f_j)$, and then $f_j=0$ for all $j\in\mathbb{Z}$, which implies

$$E_0'(X)=0.$$

$\square$

2.2 Stability of perfect nanotubes at the equilibrium

Proposition 2.4 (On assumption (H1) ii))
Under assumption (H1) i), we have

$$\mathbb{R}(L^* \times X_0^*) + \mathbb{R}\begin{pmatrix} \widehat{L^*} \\ \vdots \\ \widehat{L^*} \end{pmatrix} \quad \subset \quad Ker\, D^2_{X_0X_0}\mathcal{W}(\theta^*, L^*, X_0^*).$$

Proof of Proposition 2.4
To simplify the presentation, we set $\lambda = (\theta, L)$, $X = X_0$ and $\lambda^* = (\theta^*, L^*)$, $X^* = X_0^*$.
Step 1: Invariance by translation along L
From the explicit expression of $D_X\mathcal{W}(\lambda, X)$ given by Lemma 2.1, we see that

$$D_X\mathcal{W}(\lambda, X + \gamma\widehat{L}) = D_X\mathcal{W}(\lambda, X) \quad \text{for all } \ \gamma \in \mathbb{R}.$$

By derivation with respect to γ, we deduce in particular that

$$\begin{pmatrix} \widehat{L} \\ \vdots \\ \widehat{L} \end{pmatrix} \cdot D^2_{XX}\mathcal{W}(\lambda, X) = 0$$

which shows that $\mathbb{R}\begin{pmatrix} \widehat{L} \\ \vdots \\ \widehat{L} \end{pmatrix} \quad \subset \quad \text{Ker}\, D^2_{XX}\mathcal{W}(\lambda, X).$
Step 2: Invariance by rotation
We have

$$\mathcal{W}(\lambda, R_{\alpha,\widehat{L}}(X)) = \mathcal{W}(\lambda, X) \quad \text{for all } \ \alpha \in \mathbb{R}.$$

Taking the derivative with respect to α, we obtain

$$D_X\mathcal{W}(\lambda, R_{\alpha,\widehat{L}}(X)) \cdot (\widehat{L} \times R_{\alpha,\widehat{L}}(X)) = 0 \quad \text{for all } \ \alpha \in \mathbb{R}. \tag{2.5}$$

Taking again the derivative with respect to α at $\alpha = 0$, we obtain

$$D^2_{XX}\mathcal{W}(\lambda, X) \cdot (\widehat{L} \times X, \widehat{L} \times X) + D_X\mathcal{W}(\lambda, X) \cdot (\widehat{L} \times (\widehat{L} \times X)) = 0.$$

Using $D_X\mathcal{W}(\lambda^*, X^*) = 0$, we deduce that

$$\widehat{L^*} \times X^* \in \text{Ker}\, D^2_{XX}\mathcal{W}(\lambda^*, X^*)$$

and then

$$\mathbb{R}(L^* \times X^*) \quad \subset \quad \text{Ker}\, D^2_{XX}\mathcal{W}(\lambda^*, X^*)$$

$\square$

Proof of Proposition 1.1
Step 1: Definition and properties of ψ
We keep the notations $\lambda, X, \lambda^*, X^*$ of the proof of Proposition 2.4.
We introduce the following map

$$\psi(\lambda, X) := D_X\mathcal{W}(\lambda, X). \tag{2.6}$$

We know that $\psi(\lambda^*, X^*) = 0$, and we want to find a solution $X(\lambda)$ of $\psi(\lambda, X(\lambda)) = 0$, using an inverse function theorem. We notice that we have $D_X\psi(\lambda, X) = D^2_{XX}\mathcal{W}(\lambda, X)$, with $\ker D^2_{XX}\mathcal{W}(\lambda^*, X^*) \neq \{0\}$ by Proposition 2.4.
On the other hand we know by (2.4) and (2.1) that

$$\widehat{\mathcal{L}} \cdot \psi(\lambda, X) = 0 \quad \text{with} \quad \widehat{\mathcal{L}} := \begin{pmatrix} \widehat{L} \\ \vdots \\ \widehat{L} \end{pmatrix}$$

i.e.

$$\psi(\lambda, X) \in \widehat{\mathcal{L}}^{\perp}. \tag{2.7}$$

Moreover computation (2.5) shows that

$$\psi(\lambda, X) \in (AX)^{\perp} \quad \text{with} \quad AX := L \times X. \tag{2.8}$$

From Lemma 2.1 and Lemma 6.1, we have for all $\alpha, \gamma \in \mathbb{R}$

$$\psi(\lambda, R_{\alpha,\widehat{L}}(X) + \gamma\widehat{L}) = R_{\alpha,\widehat{L}}(\psi(\lambda, X)). \tag{2.9}$$

Step 2: Setting for invertibility
We set

$$V_1 = (A^*X^*)^{\perp} \cap \widehat{\mathcal{L}^*}^{\perp} \quad \text{with} \quad \widehat{\mathcal{L}}^* := \begin{pmatrix} \widehat{L}^* \\ \vdots \\ \widehat{L}^* \end{pmatrix} \quad \text{and} \quad A^*X^* := L^* \times A^*$$

and notice that $A^*X^* \neq 0$ because not all the atoms are aligned (as a consequence of assumption (H1) i)). We consider (with the orthogonal projection on V_1)

$$\tilde{\psi}(\lambda, \cdot) := Proj\big|_{V_1}\left(\psi(\lambda, \cdot)\big|_{X^*+V_1}\right). \tag{2.10}$$

We now want to apply the inverse function theorem to $\tilde{\psi}$. To this end, we compute

$$D_X\tilde{\psi}(\lambda^*, X^*) = Proj\big|_{V_1}\left(D^2_{XX}\mathcal{W}(\lambda^*, X^*)\big|_{V_1}\right).$$

But $D^2_{XX}\mathcal{W}(\lambda^*, X^*)$ is a symmetric matrix whose kernel is $V_1^{\perp}$ by assumption (H1) ii). Therefore $D^2_{XX}\mathcal{W}(\lambda^*, X^*)$ is invertible from V_1 to V_1, which shows the invertibility of $D_X\tilde{\psi}(\lambda^*, X^*)$.
From the inverse function theorem, there exist a bounded neighborhood $\mathcal{U}_0$ of λ^* and a bounded neighborhood $\tilde{\mathcal{V}}_0^*$ of X^* in $X^* + V_1$ and a C^1-map (because the map $(\lambda, X) \mapsto \mathcal{W}(\lambda, X)$ is C^2 by assumption (H0))

$$\begin{array}{rccc} \mathcal{X}_0^* & : & \mathcal{U}_0 & \to & \tilde{\mathcal{V}}_0^* \\ & & \lambda & \mapsto & \mathcal{X}_0^*(\lambda) \end{array}$$

such that the equation

$$\tilde{\psi}(\lambda, X) = 0 \quad \text{for} \quad X \in \tilde{\mathcal{V}}_0^*$$

has a unique solution which is $\mathcal{X}_0^*(\lambda)$.

Step 3: Consequences

Notice that $\tilde{\psi}(\lambda, X) = 0$ means

$$\psi(\lambda, X) - \alpha A^* X^* - \beta \widehat{\mathcal{L}}^* = 0 \quad \text{with} \quad \begin{cases} \alpha = \dfrac{(A^* X^*) \cdot \psi(\lambda, X)}{|A^* X^*|^2} \\ \beta = \dfrac{\widehat{\mathcal{L}}^* \cdot \psi(\lambda, X)}{|\widehat{\mathcal{L}}^*|^2}, \end{cases} \tag{2.11}$$

where we have substracted to ψ its orthogonal projection on $V_1^{\perp}$, namely

$$V_1^{\perp} = \mathbb{R}(A^* X^*) \overset{\perp}{\oplus} \mathbb{R}\widehat{\mathcal{L}}^*.$$

Taking respectively the scalar product with AX and $\widehat{\mathcal{L}}$ in (2.11), and using respectively (2.8) and (2.7), we get

$$\begin{cases} 0 - \alpha\,(A^* X^* \cdot AX) - \beta\,(\widehat{\mathcal{L}}^* \cdot AX) = 0 \\ 0 - \alpha\,(A^* X^* \cdot \widehat{\mathcal{L}}) - \beta\,(\widehat{\mathcal{L}}^* \cdot \widehat{\mathcal{L}}) = 0. \end{cases}$$

For

$$\Delta(L, X) := \det \begin{pmatrix} (A^* X^* \cdot AX) & (\widehat{\mathcal{L}}^* \cdot AX) \\ (A^* X^* \cdot \widehat{\mathcal{L}}) & (\widehat{\mathcal{L}}^* \cdot \widehat{\mathcal{L}}) \end{pmatrix},$$

we have

$$\Delta(L^*, X^*) = |A^* X^*|^2 |\widehat{\mathcal{L}}^*|^2 \neq 0,$$

and $\Delta(L, X) \neq 0$ for (L, X) close enough to (L^*, X^*) (which is true for $X = \mathcal{X}_0^*(\lambda)$ and $\lambda = (\theta, L) \in \mathcal{U}_0$, up to reduce $\mathcal{U}_0$). Therefore $\alpha = \beta = 0$ which implies that

$$\psi(\lambda, X) = 0 \quad \text{for all } X = \mathcal{X}_0^*(\lambda) \quad \text{and} \quad \lambda \in \mathcal{U}_0.$$

Step 4: Further properties

With notation (1.12), recall that not all the atoms in the nanotube $\mathcal{X}^*(\lambda^*)$ are aligned. Because $\mathcal{X}_0^*$ is a continuous map, we deduce that not all the atoms in $\mathcal{X}^*(\lambda)$ are aligned, for $\lambda \in \mathcal{U}_0$ with $\mathcal{U}_0$ small enough, which shows (1.12). Moreover up to reduce $\mathcal{U}_0$, we can assume (1.14), (1.15) and (1.16).

Step 5: Conclusion for the existence of $\mathcal{V}_0^*$

We define

$$\begin{array}{rrcl} \Phi & : \ (0, 2\pi) \times (\mathbb{R}^3 \backslash \{0\}) \times (X^* + V_1) \times \mathbb{R} \times \mathbb{R} & \longrightarrow & (0, 2\pi) \times (\mathbb{R}^3 \backslash \{0\}) \times (\mathbb{R}^3)^K \\ & (\theta, L, X, \alpha, \gamma) & \longmapsto & (\theta, L, R_{\alpha, \widehat{L}}(X) + \gamma \widehat{L}). \end{array}$$

We have $\Phi(\theta^*, L^*, X^*, 0, 0) = (\theta^*, L^*, X^*)$, and we compute

$$D\Phi(\theta^*, L^*, X^*, 0, 0) \cdot (\bar{\theta}, \bar{L}, \bar{X}, \bar{\alpha}, \bar{\gamma}) = (\bar{\theta}, \bar{L}, \bar{X} + \bar{\alpha}\widehat{L}^* \times X^* + \bar{\gamma}\widehat{L}^*).$$

This shows that $D\Phi$ is invertible at this point. Because Φ is C^1, we deduce from the inverse function theorem that there exists a bounded neighborhood $\mathcal{V}_0^*$ of X^* in $(\mathbb{R}^3)^K$ such that (up to reduce $\mathcal{U}_0$ and choose $\mathcal{V}_0^*$ small enough) for all $(\theta, L, X) \in \mathcal{U}_0 \times \mathcal{V}_0^*$, there exists a unique $(\theta, L, \tilde{X}, \alpha, \gamma) \in \mathcal{U}_0 \times \tilde{\mathcal{V}}_0^* \times B_r(0)$, with $B_{r_0}(0) \subset \mathbb{R}^2$ for some small $r_0 > 0$, such that

$$\Phi(\theta, L, \tilde{X}, \alpha, \gamma) = (\theta, L, X).$$

As a consequence if $(\theta, L, X) \in \mathcal{U}_0 \times \mathcal{V}_0^*$ and $\psi(\theta, L, X) = 0$, then

$$X = R_{\alpha,\widehat{L}}(\tilde{X}) + \gamma\widehat{L} \quad \text{with} \quad \tilde{X} \in X^* + V_1.$$

Therefore from (2.9), we deduce

$$\psi(\theta, L, \tilde{X}) = 0 \quad \text{with} \quad \tilde{X} \in X^* + V_1.$$

From Step 2, we deduce that

$$\tilde{X} = \mathcal{X}_0^*(\theta, L),$$

and then

$$X = R_{\alpha,\widehat{L}}(\tilde{\mathcal{X}}_0^*(\theta, L)) + \gamma\widehat{L},$$

which shows (1.11).

□

2.3 The kernel of the hessian

Proposition 2.5 (The kernel of the hessian)
We set

$$Z_j = u_1 + u_2 \times X_j^* + Y_j,$$

with $u_1,\ u_2 \in \mathbb{R}^3$, $X^* \in \mathcal{C}_*^{\theta^*,L^*}$, *with* $X^* = \mathcal{X}^*(\theta^*, L^*)$ *and for* $(\overline{\theta}, \overline{L}) \in \mathbb{R} \times \mathbb{R}^3$

$$Y := (\overline{\theta}, \overline{L}).\nabla_{(\theta,L)}\mathcal{X}^*(\theta^*, L^*), \tag{2.12}$$

where $\mathcal{X}^*$ *is defined in Proposition 1.1. Then*
i) for $Z = (Z_j)_{j\in\mathbb{Z}}$ *we have* $Z \in Ker\, E_0''(X^*)$
ii) there exists a constant $C > 0$ *such that* $|Z_j| \le C(1 + |j|)$

Proof of Proposition 2.5
Proof of i)
Action of translations
For $\mathcal{Y} = X^* + tu_1$, we have $\mathcal{Y}_{j,l} - \mathcal{Y}_{j',l'} = X_{j,l}^* - X_{j',l'}^*$ and then $E_0'(X^* + tu_1) = E_0'(X^*)$. Therefore

$$0 = \frac{d}{dt}(E_0'(X^* + tu_1))\Big|_{t=0} = E_0''(X^*) \cdot u_1$$

and finally

$$u_1 \in \operatorname{Ker} E_0''(X^*). \tag{2.13}$$

Action of rotations
For $\alpha \in \mathbb{R}$ and $\mathcal{Y} = R_{\alpha,\widehat{u}_2}(X^*)$, we have $\mathcal{Y}_{j,l} - \mathcal{Y}_{j',l'} = R_{\alpha,\widehat{u}_2}(X_{j,l}^* - X_{j',l'}^*)$, then we write

$$E_0'(R_{\alpha,\widehat{u}_2}(X^*)) = R_{\alpha,\widehat{u}_2}(E_0'(X^*)) = 0$$

where we have used Lemma 6.1 and the fact that $E_0'(X^*) = 0$.
Therefore for $\alpha = t|u_2|$, we get

$$0 = \frac{d}{dt} E_0'(R_{t|u_2|,\widehat{u}_2}(X^*))\big|_{\alpha=0} = E_0''(X^*) \cdot (u_2 \times X^*)$$

and finally

$$u_2 \times X^* \in \mathrm{Ker}\, E_0''(X^*). \tag{2.14}$$

Perturbation of $\mathcal{X}^*(\theta, L)$
We have

$$E_0'(\mathcal{X}^*(\theta, L)) = 0.$$

Therefore for $(\theta, L) = (\theta^*, L^*) + t(\bar{\theta}, \bar{L})$, we have

$$0 = \frac{d}{dt} E_0'(\mathcal{X}^*(\theta^* + t\bar{\theta}, L^* + t\bar{L})) = E_0''(\mathcal{X}^*(\theta^*, L^*)) \cdot Y,$$

with $Y = (\bar{\theta}, \bar{L}) \cdot \nabla_{(\theta,L)} \mathcal{X}^*(\theta^*, L^*)$. And finally

$$Y \in \mathrm{Ker}\, E_0''(X^*). \tag{2.15}$$

Conclusion
From (2.13), (2.14) and (2.15), we deduce that $Z \in \mathrm{Ker}\, E_0''(X^*)$.
Proof of ii)
On the one hand, from Lemma 3.4, we deduce that there exists a constant $C_1 > 0$ such that

$$|X_j^*| \leq C_1(1 + |j|) \tag{2.16}$$

On the other hand, we have

$$\mathcal{X}_j^*(\theta, L) = jL + R_{j\theta,\widehat{L}}(\mathcal{X}_0^*(\theta, L))$$

This gives

$$\begin{array}{rcl} Y_j & = & (\bar{\theta}, \bar{L}) \cdot \nabla_{(\theta,L)} \mathcal{X}_j^*(\theta^*, L^*) \\ & = & j\bar{L} + j\bar{\theta} R_{j\theta^* + \frac{\pi}{2},\widehat{L}^*}(\mathcal{X}_0^*(\theta^*, L^*)) + \left(\bar{L} \cdot \nabla_L R_{j\theta^*,\widehat{L}}\right)\Big|_{L=L^*} (\mathcal{X}_0^*(\theta^*, L^*)) \\ & + & R_{j\theta^*,\widehat{L}^*}\left((\bar{\theta}, \bar{L}) \cdot \nabla_{(\theta,L)} \mathcal{X}_0^*(\theta^*, L^*)\right), \end{array}$$

and then (using Lemma 6.4) there exists a constant C_2 such that

$$|Y_j| \leq C_2(1 + |j|). \tag{2.17}$$

From (2.16) and (2.17) we deduce that there exists a constant C such that

$$|Z_j| \leq C(1 + |j|).$$

$\square$

3 Rough rigidity estimates

The goal of this section is to prove Propositions 3.5 and 3.6 about finite differences of a single nanotube. This is done in Subsection 3.2. In Subsection 3.1, we present preliminary results about comparaison between two nanotubes, that are used in Subsection 3.2 and also later in Section 5.

3.1 Comparison between two nanotubes

Lemma 3.1 (Long distance error estimate for perfect nanotubes)
Let us consider two perfect nanotubes $X \in \widehat{\mathcal{C}}^{\theta,L}$ *and* $\bar{X} \in \widehat{\mathcal{C}}^{\bar{\theta},\bar{L}}$ *for* (θ, L), $(\bar{\theta}, \bar{L}) \in \mathcal{U}_0$ *such that*

$$\begin{cases} \sup_{\alpha=0,-1} |X_\alpha - \bar{X}_\alpha| \le \varepsilon \\ |\theta - \bar{\theta}| \le \varepsilon_0 \le \varepsilon \\ |L - \bar{L}| \le \varepsilon_0 \le \varepsilon. \end{cases}$$

Assume moreover that we can write

$$X = a + Y \quad \textit{with} \quad Y \in \mathcal{C}^{\theta,L} \quad \textit{and} \quad \inf_{\gamma\in\mathbb{R}} \sup_{0\le l\le K-1} |Y_{0,l} - \gamma L| \le c_1. \tag{3.1}$$

Then there exists a constant $C_0 = C_0(c_1) > 0$ *such that*

$$|X_j - \bar{X}_j| \le C_0(\varepsilon + \varepsilon_0|j|), \tag{3.2}$$

and there exists a constant $C_1 = C_1(j, c_1)$ *such that we have*

$$|(X_{j'} - X_j) - (\bar{X}_{j'} - \bar{X}_j)| \le C_1(\varepsilon_0 + \varepsilon|j' - j| + \varepsilon_0|j' - j|^2). \tag{3.3}$$

Error estimate (3.2) is illustrated on Figure 5.

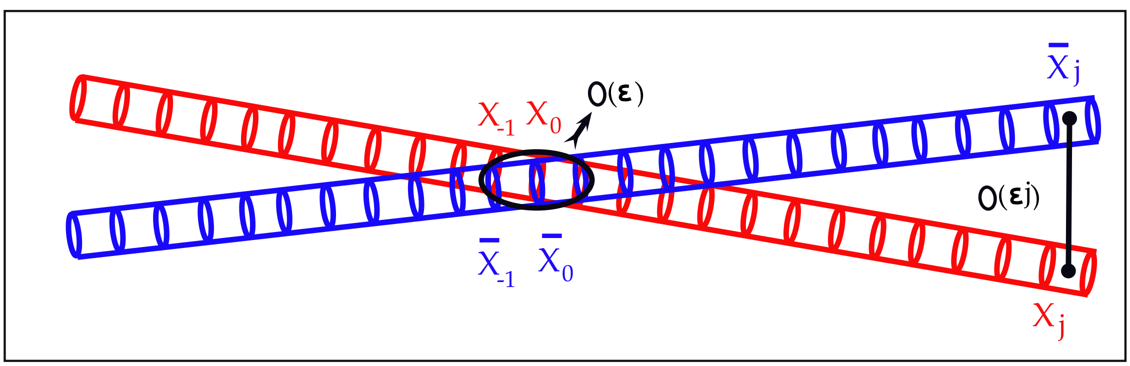

Figure 5: Illustration of error estimate (3.2)

Remark 3.2
In statement of Lemma 3.1, we assumed for simplicity that (θ, L), $(\bar{\theta}, \bar{L}) \in \mathcal{U}_0$. *Indeed the result is still true if* $|R_{\bar{\theta},\widehat{\bar{L}}} - I|$ *is bounded from bellow by a positive constant.*

Proof of Lemma 3.1
Step 1: Estimate on rotations
We have $|L-\bar{L}| \leq \varepsilon_0$, then by Lemma 6.6 there exists a constant $c>0$ such that

$$|\widehat{L}-\widehat{\bar{L}}| \leq c\varepsilon_0.$$

By Lemma 6.5, we have

$$\begin{array}{rcl} |R_{j\theta,\widehat{L}} - R_{j\bar{\theta},\widehat{\bar{L}}}| & \leq & |j\theta - j\bar{\theta}| + 5|\widehat{L}-\widehat{\bar{L}}| \\ & \leq & (|j|+5c)\varepsilon_0, \end{array}$$

where we have used the fact that $|\theta-\bar{\theta}| \leq \varepsilon_0$.
Then there exists $c_0>0$ such that (with the difference of identity matrices for $j=0$)

$$|R_{j\theta,\widehat{L}} - R_{j\bar{\theta},\widehat{\bar{L}}}| \leq c_0|j|\varepsilon_0.$$

Step 2: First estimate on $|X_j-\bar{X}_j|$
We recall that

$$\begin{cases} X_j = a + R_{j\theta,\widehat{L}}(X_0-a) + jL & \text{with} \quad a\in\mathbb{R}^3 \\ \bar{X}_j = \bar{a} + R_{j\bar{\theta},\widehat{\bar{L}}}(\bar{X}_0-\bar{a}) + j\bar{L} & \text{with} \quad \bar{a}\in\mathbb{R}^3, \end{cases}$$

where up to change a in $a+\gamma L$, we can assume that we can take $\gamma=0$ in (3.1). We have

$$|X_j-\bar{X}_j| = |(a+R_{j\theta,\widehat{L}}(X_0-a)+jL) - (\bar{a}+R_{j\bar{\theta},\widehat{\bar{L}}}(\bar{X}_0-\bar{a})+j\bar{L})|$$

and then

$$|X_j-\bar{X}_j| = |a-\bar{a}-R_{j\bar{\theta},\widehat{\bar{L}}}(a-\bar{a}) + (R_{j\theta,\widehat{L}} - R_{j\bar{\theta},\widehat{\bar{L}}})(X_0-a) + R_{j\bar{\theta},\widehat{\bar{L}}}(X_0-\bar{X}_0) + j(L-\bar{L})| \tag{3.4}$$

This implies

$$\begin{array}{rcl} |X_j-\bar{X}_j| & \leq & |a-\bar{a}-R_{j\bar{\theta},\widehat{\bar{L}}}(a-\bar{a})| + |R_{j\theta,\widehat{L}} - R_{j\bar{\theta},\widehat{\bar{L}}}||X_0-a| + |X_0-\bar{X}_0| + |j||L-\bar{L}| \\ & \leq & A_j + c_1c_0|j|\varepsilon_0 + \varepsilon + |j|\varepsilon_0, \end{array}$$

with

$$A_j = |a-\bar{a}-R_{j\bar{\theta},\widehat{\bar{L}}}(a-\bar{a})|.$$

This gives

$$|X_j-\bar{X}_j| \leq A_j + c_4(\varepsilon+\varepsilon_0|j|), \tag{3.5}$$

with $c_4=\max(1,c_1c_0+1)$.
Step 3: Control of A_1
Again from (3.4), we get (using $\varepsilon_0\leq\varepsilon$)

$$A_j \leq |X_j-\bar{X}_j| + c_4(1+|j|)\varepsilon.$$

For $j=1$, this gives

$$A_1 \leq \varepsilon + 2c_4\varepsilon \leq c_5\varepsilon,$$

with $c_5 = 1 + 2c_4$.

Step 4: Control of A_j

We get with $u = a - \bar{a}$

$$A_1 = |u - R_{\bar{\theta},\widehat{\bar{L}}}(u)| \le c_5\varepsilon. \tag{3.6}$$

Let $u^\perp = u - (u \cdot \widehat{\bar{L}})\widehat{\bar{L}}$. Then using (3.6) and $(\bar{\theta}, \bar{L}) \in \mathcal{U}_0$ which implies that $|R_{\bar{\theta},\widehat{\bar{L}}} - I|$ is bounded from below by some positive constant, there exists $c_6 > 0$ such that

$$|u^\perp| \le c_6\varepsilon,$$

and for all $j \in \mathbb{Z}$

$$A_j = |u - R_{j\bar{\theta},\widehat{\bar{L}}}(u)| = |u^\perp - R_{j\bar{\theta},\widehat{\bar{L}}}(u^\perp)| \le 2c_6\varepsilon.$$

Step 5: Conclusion

Similarly we get

$$|X_j - \bar{X}_j| \le A_j + c_4(\varepsilon + \varepsilon_0|j|) \le 2c_6\varepsilon + c_4(\varepsilon + \varepsilon_0|j|) \le C(\varepsilon + \varepsilon_0|j|),$$

with $C = 2c_6 + c_4$, which shows (3.2).

Step 6: Bound on $|(X_{j'} - X_j) - (\bar{X}_{j'} - \bar{X}_j)|$

We compute (using (3.2)),

$$\begin{aligned} |(X_{k+1} - \bar{X}_{k+1}) - (X_k - \bar{X}_k)| &\le C(\varepsilon + \varepsilon_0|k+1|) + C(\varepsilon + \varepsilon_0|k|) \\ &\le C_1(\varepsilon + \varepsilon_0|k|). \end{aligned} \tag{3.7}$$

Up to change (j, j') in $(-j, -j')$ we can assume that $j' > j$. Then by iteration of (3.7), we have

$$|(X_{j'} - X_j) - (\bar{X}_{j'} - \bar{X}_j)| \le C_1 \left(\varepsilon|j' - j| + \varepsilon_0 \sum_{k=j}^{j'-1} |k| \right) \quad \text{for } j' > j. \tag{3.8}$$

We distinguish the cases

$$\sum_{k=j}^{j'-1} |k| = \begin{cases} \displaystyle\sum_{k=j}^{j'-1} k & \text{if } \ j \ge 0 \\ \displaystyle -\sum_{k=1-j'}^{j} k & \text{if } \ j' - 1 \le 0 \\ \displaystyle -\sum_{k=j}^{0} k + \sum_{k=0}^{j'-1} k & \text{if } \ j < 0 < j' - 1. \end{cases}$$

In each case, we deduce that there exists a constant $c_7 = c_7(j)$ such that we have

$$\sum_{k=j}^{j'-1} |k| \le c_7(1 + |j' - j|^2),$$

Joint to (3.8), we deduce that there exists a constant $C_2 = C_2(j)$ such that we have

$$|(X_{j'} - X_j) - (\bar{X}_{j'} - \bar{X}_j)| \le C_2(\varepsilon_0 + \varepsilon|j' - j| + \varepsilon_0|j' - j|^2).$$

$\square$

Lemma 3.3 (Estimate between a general and a perfect nanotube)
Let us consider a nanotube X and $(\theta_0, L_0) \in \mathcal{U}_0$. Let us assume that we have

$$\sup_{|\alpha|\le 1} |X_\alpha - \widehat{X}^*_\alpha| \le \varepsilon \quad \textit{with} \quad \widehat{X}^* \in \widehat{\mathcal{C}}^{\theta_0,L_0}_*.$$

Let us assume the existence of sequences $(\theta_j, L_j) \in \mathcal{U}_0$ such that for some $\varepsilon > 0$, we have

$$D_j(X,\theta_j,L_j) \le \varepsilon \quad \textit{for } M \le j \le N \quad \textit{with } M \le 0 \le N \tag{3.9}$$

and for some $\varepsilon_0 \ge 0$

$$\left\{ \begin{array}{l} |\theta_{j+1} - \theta_j| \le \varepsilon_0 \le \varepsilon \\ |L_{j+1} - L_j| \le \varepsilon_0 \le \varepsilon \end{array} \right| \qquad \textit{for } M \le j \le N-1.$$

Then there exists a constant $c > 0$ such that

$$|X_j - \widehat{X}^*_j| \le c\big(\varepsilon(1+|j|) + \varepsilon_0 j^2\big) \quad \textit{for} \quad M \le j \le N. \tag{3.10}$$

Error estimate (3.10) is illustrated on Figure 6.

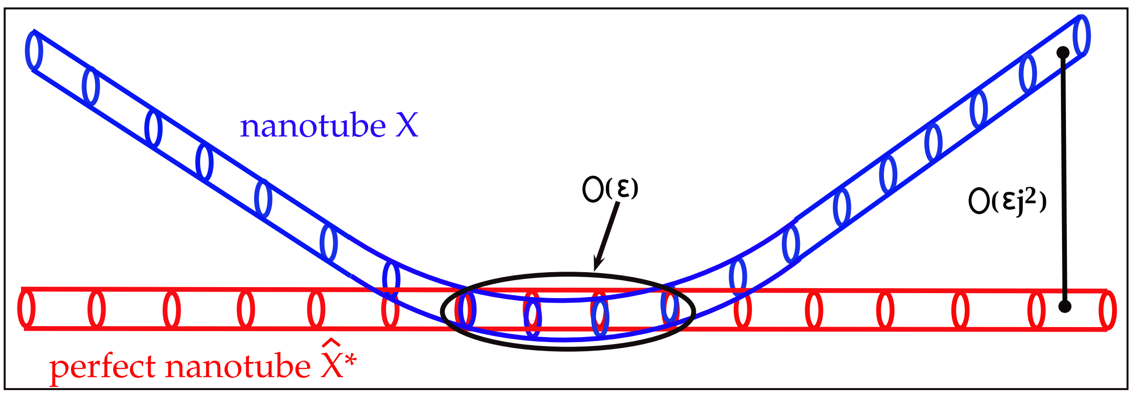

Figure 6: Illustration of error estimate (3.10) between a general and a perfect nanotube

Proof of Lemma 3.3
Let us consider a perfect nanotube $\widehat{X}^{*,j} \in \widehat{\mathcal{C}}^{\theta_j,L_j}$ that achieves the infimum in $D_j(X,\theta_j,L_j)$, which satisfies in particular

$$\sup_{|\alpha|\le 1} |X_{j+\alpha} - \widehat{X}^{*,j}_{j+\alpha}| \le \varepsilon,$$

with the choice $\widehat{X}^{*,0} := \widehat{X}^*$.
We see that (3.9) implies for $M \le j \le N$

$$\left\{ \begin{array}{l} |X_j - \widehat{X}^{*,j}_j| \le \varepsilon \\ |X_{j+1} - \widehat{X}^{*,j}_{j+1}| \le \varepsilon \\ |X_{j-1} - \widehat{X}^{*,j}_{j-1}| \le \varepsilon. \end{array} \right. \tag{3.11}$$

Similarly for j replaced by $j-1$ with $M \le j-1 \le N$, we have

$$\left\{ \begin{array}{l} |X_{j-1} - \widehat{X}^{*,j-1}_{j-1}| \le \varepsilon \\ |X_j - \widehat{X}^{*,j-1}_j| \le \varepsilon \\ |X_{j-2} - \widehat{X}^{*,j-1}_{j-2}| \le \varepsilon. \end{array} \right. \tag{3.12}$$

Using the first line in (3.11) and the second line in (3.12) , we get

$$|\widehat{X}_j^{*,j} - \widehat{X}_j^{*,j-1}| \leq 2\varepsilon. \tag{3.13}$$

Using the last line in (3.11) and the first line in (3.12) , we get

$$|\widehat{X}_{j-1}^{*,j} - \widehat{X}_{j-1}^{*,j-1}| \leq 2\varepsilon. \tag{3.14}$$

We summarize (3.13) and (3.14) as

$$\sup_{\alpha=0,-1} |\widehat{X}_{j+\alpha}^{*,j} - \widehat{X}_{j+\alpha}^{*,j-1}| \leq 2\varepsilon \quad \text{for } M+1 \leq j \leq N.$$

Because we have $|\theta_j - \theta_{j-1}| \leq \varepsilon_0$ and $|L_j - L_{j-1}| \leq \varepsilon_0$, using (3.2) in Lemma 3.1 then there exists $c_0 = 2C_0 > 0$ such that we have

$$|\widehat{X}_k^{*,j} - \widehat{X}_k^{*,j-1}| \leq c_0(\varepsilon + \varepsilon_0|j-k|). \tag{3.15}$$

Therefore, we can write for $0 \leq j \leq N$

$$\begin{array}{rcl} |\widehat{X}_j^{*,j} - \widehat{X}_j^{*,0}| & = & |(\widehat{X}_j^{*,j} - \widehat{X}_j^{*,j-1}) + (\widehat{X}_j^{*,j-1} - \widehat{X}_j^{*,j-2}) + ... + (\widehat{X}_j^{*,1} - \widehat{X}_j^{*,0})| \\ & \leq & |\widehat{X}_j^{*,j} - \widehat{X}_j^{*,j-1}| + |\widehat{X}_j^{*,j-1} - \widehat{X}_j^{*,j-2}| + ... + |\widehat{X}_j^{*,1} - \widehat{X}_j^{*,0}| \\ & \leq & c_0\big((\varepsilon + 0\varepsilon_0) + (\varepsilon + 1\varepsilon_0) + ... + (\varepsilon + |j-1|\varepsilon_0)\big) \\ & \leq & c_0(\varepsilon|j| + \varepsilon_0 j^2), \end{array} \tag{3.16}$$

where in the third line we have used (3.15). Similarly we get the same result for $M \leq j \leq 0$ and then for $M \leq j \leq N$. Finally, we have for $M \leq j \leq N$

$$\begin{array}{rcl} |X_j - \widehat{X}_j^*| & \leq & |X_j - \widehat{X}_j^{*,j}| + |\widehat{X}_j^{*,j} - \widehat{X}_j^*| \\ & = & |X_j - \widehat{X}_j^{*,j}| + |\widehat{X}_j^{*,j} - \widehat{X}_j^{*,0}| \\ & \leq & \varepsilon + c_0(\varepsilon|j| + \varepsilon_0 j^2) \\ & \leq & c(\varepsilon(1+|j|) + \varepsilon_0 j^2), \end{array}$$

with $c = \max\{1, c_0\}$ and where in the third line we have used (3.16) and the first line of (3.11).

□

3.2 Finite differences for a single nanotube

In order to prove Propositions 3.5 and 3.6 we need first the following result:

Lemma 3.4 (Estimate on perfect nanotubes)
For $(\theta, L) \in \mathcal{U}_0$, let us consider $X \in \mathcal{C}^{\theta,L}$. Then we have

$$|X_{j',l'} - X_{j,l} - (j'-j)L| \leq 4C_0, \tag{3.17}$$

with $C_0 = \inf_{\gamma \in \mathbb{R}} \sup_{0 \leq l \leq K-1} |X_{0,l} - \gamma L|$.

Proof of Lemma 3.4
We have

$$\begin{aligned} X_{j,l} - X_{j',l'} &= jL + R_{j\theta,\widehat{L}}(X_{0,l}) - j'L - R_{j'\theta,\widehat{L}}(X_{0,l'}) \\ &= (j-j')L + (R_{j\theta,\widehat{L}} - R_{j'\theta,\widehat{L}})(X_{0,l}) + R_{j'\theta,\widehat{L}}(X_{0,l} - X_{0,l'}), \\ &= (j-j')L + (R_{j\theta,\widehat{L}} - R_{j'\theta,\widehat{L}})(X_{0,l} - V) + R_{j'\theta,\widehat{L}}((X_{0,l} - V) - (X_{0,l'} - V)), \end{aligned}$$

for any vector $V = \gamma L$ for $\gamma \in \mathbb{R}$. We deduce that (3.17) holds.

$\square$

Proposition 3.5 (Estimate on a general nanotube)
There exists a constant C such that the following holds.
For any general nanotube X, $(\theta, L) \in \mathcal{U}_0$ and $\delta \in (0,1)$, satisfying

$$\sup_{j\in\mathbb{Z}} D_j(X,\theta,L) \leq \delta,$$

we have

$$|X_{j',l'} - X_{j,l} - (j'-j)L| \leq C(1 + \delta|j'-j|). \tag{3.18}$$

Moreover there exists $\widehat{X}^{*,j} \in \widehat{\mathcal{C}}^{\theta,L}$ such that

$$|X_{j',l'} - X_{j,l} - (\widehat{X}^{*,j}_{j',l'} - \widehat{X}^{*,j}_{j,l})| \leq C\delta(1 + |j'-j|). \tag{3.19}$$

Proof of Proposition 3.5
We recall that there exists $\widehat{X}^{*,j} \in \widehat{\mathcal{C}}^{\theta,L}_*$ such that

$$D_j(X,\theta,L) = \sup_{|\alpha|\leq q} |X_{j+\alpha} - \widehat{X}^{*,j}_{j+\alpha}| \leq \delta \tag{3.20}$$

Writing $\widehat{X}^{*,j} = X^{*,j} + a_j$ with $X^{*,j} \in \mathcal{C}^{\theta,L}_*$ and $a_j \in L^\perp$, we deduce from Lemma 3.4 that there exists a constant C_1 such that

$$|X^{*,j}_{j,l} - X^{*,j}_{j',l'} - (j-j')L| \leq C_1. \tag{3.21}$$

Because of (3.20), we can apply (3.10) in Lemma 3.3 with $\varepsilon_0 = 0$, and get the existence of a constant C_2 such that we have

$$|X_{j',l'} - X^{*,j}_{j',l'}| \leq C_2\delta(1 + |j-j'|) \quad \text{for all } j \in \mathbb{Z}.$$

In particular for $(j',l') = (j,l)$, we get

$$|X_{j,l} - X^{*,j}_{j,l}| \leq C_2\delta,$$

Subtracting the two last lines, we get that there exists a constant C_3 such that

$$|X_{j,l} - X_{j',l'} - (X^{*,j}_{j,l} - X^{*,j}_{j',l'})| \leq C_3\delta(1 + |j-j'|),$$

which shows (3.19).
Using (3.21), we see that there exists a constant C_4 such that we have

$$|X_{j,l} - X_{j',l'} - (j-j')L| \leq C_4(1 + \delta|j-j'|). \tag{3.22}$$

$\square$

Proposition 3.6 (Another estimate on a general nanotube)
There exist $\eta \in (0,1)$ and $C_0 > 0$ such that the following holds. Let us consider $(\theta, L) \in \mathcal{U}_0$, $\delta \in (0,\eta)$ and a nanotube X, satisfying

$$\sup_{j\in\mathbb{Z}} D_j(X,\theta,L) \le \delta,$$

such that for some $(\theta^0, L^0) \in \mathcal{U}_0$, there exists $\widehat{X}^* \in \widehat{\mathcal{C}}_*^{\theta^0,L^0}$ satisfying

$$\sup_{|\alpha|\le q} |X_\alpha - \widehat{X}^*_\alpha| \le \delta.$$

Then for $t \in [0,1]$

$$Z_{j,l}(t) = tX_{j,l} + (1-t)\widehat{X}^*_{j,l},$$

we have

$$|Z_{j,l}(t) - Z_{j',l'}(t)| \ge C_0|j'-j| \quad \textit{if} \quad |j-j'| \ge \frac{1}{C_0}. \tag{3.23}$$

Proof of Proposition 3.6
From Lemma 3.4 and Proposition 3.5, we get respectively

$$|\widehat{X}^*_{j,l} - \widehat{X}^*_{j',l'} - (j-j')L^0| \le C_1, \tag{3.24}$$

and

$$|X_{j,l} - X_{j',l'} - (j-j')L| \le C_2(1+\delta|j-j'|). \tag{3.25}$$

with C_1, $C_2 > 0$. If we multiply (3.24) by $1-t$ and (3.25) by t, we can deduce that

$$\begin{array}{rcl} |Z_{j,l}(t) - Z_{j',l'}(t) - (tL+(1-t)L^0)(j-j')| & \le & tC_2(1+\delta|j-j'|) + (1-t)C_1 \\ & \le & C_3\delta|j-j'| + C_3, \end{array}$$

with $C_3 > 0$. We can write

$$tL + (1-t)L^0 = L + (1-t)(L^0 - L).$$

We compute

$$|Z_{j,l}(t) - Z_{j',l'}(t) - (j-j')L)| \le C_3\delta|j-j'| + C_3 + |j-j'||L^0-L|.$$

This implies

$$\begin{array}{rcl} |Z_{j,l}(t) - Z_{j',l'}(t)| & \ge & |j-j'||L| - C_3 - |j-j'||L^0-L| - C_3\delta|j-j'| \\ & = & |j-j'|(|L| - |L^0-L| - C_3\delta) - C_3. \end{array}$$

Recall that we have from (1.15)

$$|L| - |L^0 - L| \ge c_0 > 0.$$

Therefore

$$|L| - |L^0-L| - C_3\delta \ge \frac{c_0}{2} \quad \text{for} \quad \delta \le \eta := \frac{c_0}{2C_3},$$

and we deduce that there exist constants C_4 and C_5 such that we have

$$|Z_{j,l}(t) - Z_{j',l'}(t)| \ge C_4|j-j'| - C_5.$$

Then there exists a constant $C_0 > 0$ such that if $|j-j'| \ge \dfrac{1}{C_0}$, we have

$$|Z_{j,l}(t) - Z_{j',l'}(t)| \ge C_0|j-j'|. \tag{3.26}$$

□

4 Fine rigidity results for nanotubes

The main result of this section is the following:

Theorem 4.1 (Main rigidity estimate)
There exists a constant $C > 0$, such that for every nanotube X, and any $\varepsilon \in (0,1)$, if

$$\inf_{(\theta,L)\in\mathcal{U}_0} D_j(X,\theta,L) \le \varepsilon \qquad \text{for } M \le j \le N \quad \text{with } M < 0 < N,$$

then the following holds.
If for some $(\theta^0, L^0) \in \mathcal{U}_0$, we have $\widehat{X}^* \in \widehat{\mathcal{C}}_*^{\theta^0,L^0}$ and $\sup_{|\alpha|\le q} |X_\alpha - \widehat{X}_\alpha^*| \le \varepsilon$.
Then $\bar{X} := X - \widehat{X}^*$ satisfies

$$|\bar{X}_j| \le C\varepsilon(1 + |j|^2) \qquad \text{for} \quad M \le j \le N, \tag{4.1}$$

and for all $M + 1 \le j \le N - 1$, there exists a constant $C' = C'(j)$ such that we have

$$|\bar{X}_{j'} - \bar{X}_j| \le C'\varepsilon(1 + |j' - j|^2) \qquad \text{for all} \quad M \le j' \le N. \tag{4.2}$$

In order to prove our main result we need Lemma 4.2 and Proposition 4.4.

Lemma 4.2 (A quantitative estimate for perfect nanotubes)
Assume that $X \in \widehat{\mathcal{C}}^{\theta,L}$, $\bar{X} \in \widehat{\mathcal{C}}^{\bar{\theta},\bar{L}}$, with (θ, L), $(\bar{\theta}, \bar{L}) \in [0, 2\pi) \times (\mathbb{R}^3\backslash\{0\})$, with

$$\begin{cases} \sup_{\alpha=0,1} |\bar{X}_\alpha - X_\alpha| \le \varepsilon \\ |\widehat{\bar{L}} - \widehat{L}| \le \varepsilon. \end{cases} \tag{4.3}$$

If moreover

$$X = a + Y \quad \text{with} \quad Y \in \mathcal{C}^{\theta,L}$$

and

$$\begin{cases} \inf_{\gamma\in\mathbb{R}} \sup_{0\le l\le K-1} |Y_{0,l} - \gamma L| \le c_1 \\ |L| \le c_1, \end{cases} \tag{4.4}$$

then there exists $C = C(c_1) > 0$, such that

$$\big||L| - |\bar{L}|\big| \le C\,\varepsilon. \tag{4.5}$$

Proof of Lemma 4.2
We recall that

$$X_1 - a = R_{\theta,\widehat{L}}(X_0 - a) + L,$$

and then

$$\widehat{L} \cdot (X_1 - X_0) = |L|, \tag{4.6}$$

and similarly

$$\widehat{\bar{L}} \cdot (\bar{X}_1 - \bar{X}_0) = |\bar{L}|. \tag{4.7}$$

From (4.3), we deduce

$$|(\bar{X}_1 - \bar{X}_0) - (X_1 - X_0)| \leq 2\varepsilon.$$

Taking the scalar product with $\widehat{\bar{L}}$, we get

$$|\widehat{\bar{L}} \cdot (\bar{X}_1 - \bar{X}_0) - \widehat{\bar{L}} \cdot (X_1 - X_0)| \leq 2\varepsilon.$$

i.e. (using (4.7))

$$||\bar{L}| - \widehat{\bar{L}} \cdot (X_1 - X_0)| \leq 2\varepsilon.$$

Using moreover (4.6), we deduce

$$||\bar{L}| - |L|| \leq 2\varepsilon + |(X_1 - X_0) \cdot (\widehat{\bar{L}} - \widehat{L})|.$$

We also have for any $\gamma \in \mathbb{R}$

$$X_1 - X_0 = L + (R_{\theta,\widehat{L}} - I)(Y_0 - \gamma L),$$

and (4.4) implies

$$||\bar{L}| - |L|| \leq 2\varepsilon + 3c_1\varepsilon,$$

which implies (4.5).

□

In order to prove Proposition 4.4 below, we need to introduce the following:

Definition 4.3 (Barycenter and centered cell)
We define the barycenter b_j of the cell X_j of a nanotube $X = ((X_{j,l})_{0\leq l\leq K-1})_{j\in\mathbb{Z}}$ by

$$b_j = \frac{1}{K}\sum_{l=0}^{K-1} X_{j,l}.$$

And we define the centered cell X'_j by

$$X'_{j,l} = X_{j,l} - b_j \quad \text{and} \quad X'_j = (X'_{j,l})_{0\leq l\leq K-1}.$$

Proposition 4.4 (Error estimate on the angles and the axes)
There exists a constant $C > 0$ and $\varepsilon_1 > 0$ such that if a nanotube X satisfies for some $\varepsilon \in [0, \varepsilon_1)$

$$D_k(X, \theta_k, L_k) \leq \varepsilon \quad \text{for } k = j,\ j+1,$$

then we have

$$\left\{ \begin{array}{l} |\theta_{j+1} - \theta_j| \leq C\varepsilon \\ |L_{j+1} - L_j| \leq C\varepsilon. \end{array} \right. \tag{4.8}$$

Proof of Proposition 4.4
We have

$$D_k(X, \theta_k, L_k) \leq \varepsilon \quad \text{for } k = j,\ j+1,$$

which implies that there exists $\widehat{X}^{*,k} \in \widehat{\mathcal{C}}_*^{\theta_k, L_k}$ such that

$$\sup_{|\alpha|\leq q} |X_{k+\alpha} - \widehat{X}^{*,k}_{k+\alpha}| \leq \varepsilon. \tag{4.9}$$

Taking the difference for $k = j$ and $\alpha = 0, 1$ (respectively $k = j + 1$ and $\alpha = -1, 0$), we get

$$\sup_{\beta=0,1} |\widehat{X}^{*,j+1}_{j+\beta} - \widehat{X}^{*,j}_{j+\beta}| \leq 2\varepsilon. \tag{4.10}$$

Step 1: Preliminary estimate
Writing

$$\widehat{X}^{*,k} = a_k + X^{*,k} \quad \text{with} \quad X^{*,k} \in \mathcal{C}_*^{\theta_k, L_k} \quad \text{and} \quad \left\{ \begin{array}{l} \inf\limits_{\gamma\in\mathbb{R}} \sup\limits_{0\leq l\leq K-1} |X^{*,k}_{k,l} - \gamma L_k| \leq c_1 \\ |L_k| \leq c_1, \end{array} \right. \tag{4.11}$$

with $c_1 > 0$, we deduce (by convexity) for the centered cell (see Definition 4.3)

$$\sup_{\beta=0,1} |(X^{*,j+1}_{j+\beta})' - (X^{*,j}_{j+\beta})'| \leq 2\varepsilon. \tag{4.12}$$

Applying the rotation $R_{\theta_{j+1},\widehat{L}_{j+1}}$ to (4.12) for $\beta = 0$, we get

$$|R_{\theta_{j+1},\widehat{L}_{j+1}}(X^{*,j+1}_j)' - R_{\theta_{j+1},\widehat{L}_{j+1}}(X^{*,j}_j)'| \leq 2\varepsilon. \tag{4.13}$$

Recall that

$$(X^{*,k}_{j+1})' = R_{\theta_k,\widehat{L}_k}(X^{*,k}_j)'.$$

Then (4.12) for $\beta = 1$ can be rewritten as

$$|R_{\theta_{j+1},\widehat{L}_{j+1}}(X^{*,j+1}_j)' - R_{\theta_j,\widehat{L}_j}(X^{*,j}_j)'| \leq 2\varepsilon. \tag{4.14}$$

Substracting (4.13) and (4.14), we get

$$|(R_{\theta_{j+1},\widehat{L}_{j+1}} - R_{\theta_j,\widehat{L}_j})(X^{*,j}_j)'| \leq 4\varepsilon. \tag{4.15}$$

Step 2: Estimate on $|(\theta_{j+1}, \widehat{L}_{j+1}) - (\theta_j, \widehat{L}_j)|$
Case 1: $q \geq 1$ and three atoms of $\mathcal{X}_0^*(\theta, L)$ are not aligned for each $(\theta, L) \in \mathcal{U}_0$
Because we can find at least three atoms not aligned in $X^{*,j}_j$, this implies that there exist two vectors v_i, $i = 1, 2$ in the centered cell $(X^{*,j}_j)'$ such that

$$|v_1|, |v_2| \leq \frac{1}{c_0} \quad \text{and} \quad |v_1 \times v_2| \geq c_0 > 0, \tag{4.16}$$

for some constant c_0 uniform in $(\theta_j, L_j) \in \mathcal{U}_0$.
If $\theta_j \in [0, \pi]$, using the fact that

$$\overline{\mathcal{U}_0} \subset (0, 2\pi) \times \mathbb{R}^3 \backslash \{0\}, \tag{4.17}$$

then we can apply Lemma 6.7 to (4.15) and deduce that there exists a constant $C_1 > 0$ and $m \in \mathbb{Z}$ such that

$$\left\{ \begin{array}{l} |\theta_{j+1} - \theta_j - 2m\,\pi| \leq C_1\varepsilon \\ |\widehat{L}_{j+1} - \widehat{L}_j| \leq C_1\varepsilon. \end{array} \right. \tag{4.18}$$

or (using $R_{2\pi-\theta_{j+1},-\widehat{L}_{j+1}} = R_{\theta_{j+1},\widehat{L}_{j+1}}$)

$$\left\{ \begin{array}{l} |2\,\pi - \theta_{j+1} - \theta_j - 2m\,\pi| \leq C_1\varepsilon \\ | - \widehat{L}_{j+1} - \widehat{L}_j| \leq C_1\varepsilon. \end{array} \right. \tag{4.19}$$

The last line of (4.19) is impossible for $(\theta_k, L_k) \in \mathcal{U}_0$, $k = j, j+1$ and ε small enough, because of (1.15). Notice that (4.17) implies $m = 0$ for ε in (4.18) small enough. Similarly if $\theta_j \in [\pi, 2\pi]$, we set $\bar{\theta}_k = 2\pi - \theta_k$, $\bar{L}_k = -L_k$ for $k = j, j+1$ and apply the previous reasoning to $\bar{\theta}_j \in [0, \pi]$. Then in all cases this shows

$$\begin{cases} |\theta_{j+1} - \theta_j| \le C_1 \varepsilon \\ |\widehat{L}_{j+1} - \widehat{L}_j| \le C_1 \varepsilon. \end{cases} \tag{4.20}$$

Case 2: The general case

Let us consider the new supercell $\tilde{X}_0^{*,k}$ (see Figure 7) for $k = j, j+1$ built from the r cells $X_j^{*,k}$, $X_{j+1}^{*,k}, ..., X_{j+r-1}^{*,k}$ for $r \ge 2$, with

$$\tilde{X}_m^{*,k} = (\tilde{X}_{m,\tilde{l}}^{*,k})_{0 \le \tilde{l} \le \tilde{K}-1} \quad \text{with} \quad \tilde{K} = rK, \ \tilde{X}_{m,pK+l}^{*,k} = X_{j+mr+p,l}^{*,k} \quad \text{for} \quad p = 0, ..., r-1 \quad \text{and} \quad l = 0, ..., K-1.$$

Because $X^{*,k} \in \mathcal{C}^{\theta_k, L_k}$, we get $\tilde{X}^{*,k} \in \mathcal{C}^{\tilde{\theta}_k, \tilde{L}_k}$ with $\tilde{\theta}_k = r\theta_k$ and $\tilde{L}_k = rL_k$, and $\tilde{X}^{*,k}$ satisfies

$$\tilde{X}_{m+1}^{*,k} = R_{\tilde{\theta}_k, \widehat{\tilde{L}}_k}(\tilde{X}_m^{*,k}) + \tilde{L}_k.$$

Now if all the atoms of $\tilde{X}_0^{*,k}$ are aligned, applying T^{θ_k, L_k} to the cells $X_j^{*,k}$, $X_{j+1}^{*,k}, ..., X_{j+r-1}^{*,k}$, we get that all the atoms of $X_{j+1}^{*,k}$, $X_{j+2}^{*,k}, ..., X_{j+r}^{*,k}$ are also aligned.
If $r \ge 3$, whatever is the value $K \ge 1$, we conclude that all the atoms of $X_j^{*,k}$, $X_{j+1}^{*,k}, ..., X_{j+r}^{*,k}$ are aligned.

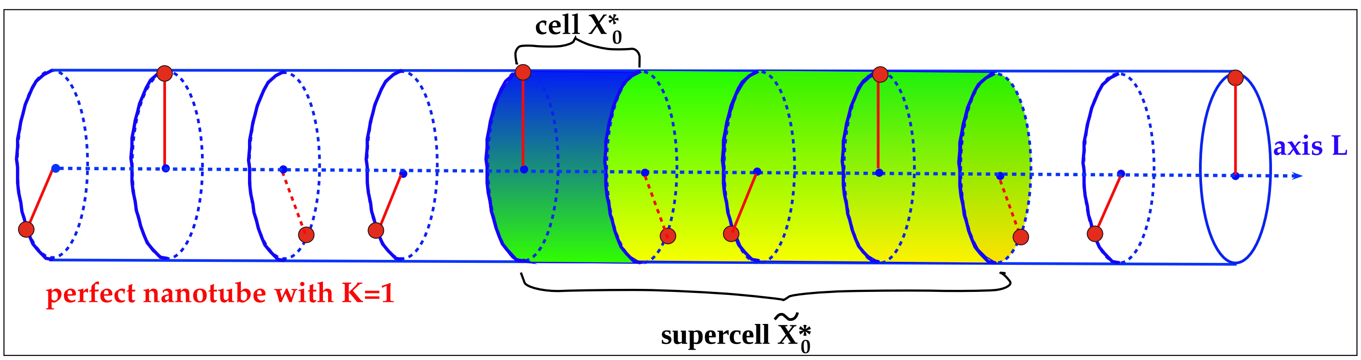

Figure 7: The supercell $\tilde{X}_0^*$ constructed using $X_0^*, ..., X_{r-1}^*$ for $r = 4$, $\theta = \dfrac{2\pi}{3}$, and $K = 1$

If $K \ge 2$ and $r \ge 2$, we also conclude that all the atoms of $X_j^{*,k}, ..., X_{j+r}^{*,k}$ are aligned.
By iteration, this implies that all atoms of $X^{*,k}$ are aligned, which is excluded by assumption (1.13). We conclude that we can find three atoms not aligned in $\tilde{X}_0^{*,k}$.
Recalling the definition of a_k in (4.11), we define

$$\widehat{\tilde{X}}_m^{*,k} := a_k + \tilde{X}_m^{*,k}.$$

Following assumption (H3), and using (1.16), we get that $r\theta \ne 0\,(2\pi)$ for all $(\theta, L) \in \mathcal{U}_0$.
Recall that (4.9) implies (by difference) for $k = j$ and $k = j+1$ and $q \ge q_0 \ge 2r-1 \ge r \ge 1$

$$|\widehat{X}_{j+\beta}^{*,j+1} - \widehat{X}_{j+\beta}^{*,j}| \le 2\varepsilon \quad \text{for} \quad 0 \le \beta \le 2r-1.$$

This implies

$$|\widehat{\tilde{X}}^{*,j+1}_{\tilde{\beta}} - \widehat{\tilde{X}}^{*,j}_{\tilde{\beta}}| \leq 2\varepsilon \quad \text{for} \quad \tilde{\beta} = 0,1, \tag{4.21}$$

which is exactly similar to (4.10).
This shows that we can apply Step 1 and Step 2 (case 1) using (4.21) in place of (4.10). Because by construction there are at least three atoms not aligned in the centered cell $(\tilde{X}_j^{*,j})'$ with $\tilde{\theta}_j = r\theta_j \neq 0\,(2\,\pi)$ and $\tilde{L}_j = rL_j$, we conclude that

$$\left\{ \begin{array}{l} |\tilde{\theta}_{j+1} - \tilde{\theta}_j| \leq C_1\varepsilon \\ |\widehat{\tilde{L}}_{j+1} - \widehat{\tilde{L}}_j| \leq C_1\varepsilon, \end{array} \right.$$

which implies (4.20).
Step 3: Proof of $|L_{j+1} - L_j| \leq C\varepsilon$.
Because

$$|\widehat{L}_{j+1} - \widehat{L}_j| \leq C_1\varepsilon, \tag{4.22}$$

we can apply Lemma 4.2, using (4.10) and (4.11) and checking that (4.4) is satisfied because $(\theta_j, L_j) \in \mathcal{U}_0$. We deduce that there exists a constant C_2 such that

$$\big||L_{j+1}| - |L_j|\big| \leq C_2\varepsilon. \tag{4.23}$$

We can compute

$$\begin{array}{rcl} |L_{j+1} - L_j| & = & \big||L_{j+1}|\widehat{L}_{j+1} - |L_j|\widehat{L}_j\big| \\ & = & \big||L_{j+1}|\widehat{L}_{j+1} - |L_{j+1}|\widehat{L}_j + |L_{j+1}|\widehat{L}_j - |L_j|\widehat{L}_j\big| \\ & \leq & |L_{j+1}||\widehat{L}_{j+1} - \widehat{L}_j| + \big||L_{j+1}| - |L_j|\big||\widehat{L}_j|. \end{array}$$

Using (4.23) and (4.22), we deduce that there exists a constant C_3 such that

$$|L_{j+1} - L_j| \leq C_3\varepsilon,$$

This last inequality and (4.20) imply (4.8).

$\square$

Proof of Theorem 4.1
Step 1: Proof of (4.1)
We have

$$\left\{ \begin{array}{l} \displaystyle\inf_{(\theta,L)\in\mathcal{U}_0} D_j(X,\theta,L) \leq \varepsilon \qquad \text{for } M \leq j \leq N \\ \displaystyle\sup_{|\alpha|\leq q} |X_\alpha - \widehat{X}^*_\alpha| \leq \varepsilon, \end{array} \right.$$

then for $M \leq j \leq N$, there exists $(\theta_j, L_j) \in \mathcal{U}_0$ such that

$$\left\{ \begin{array}{l} D_j(X,\theta_j,L_j) \leq \varepsilon \\ \text{with } \theta_0 = \theta^0 \text{ and } L_0 = L^0. \end{array} \right. \tag{4.24}$$

Then by Proposition 4.4 we deduce that there exists a constant $c > 0$ such that we have

$$\left\{ \begin{array}{l} |\theta_{j+1} - \theta_j| \leq c\varepsilon \\ |L_{j+1} - L_j| \leq c\varepsilon \end{array} \right| \text{for } M \leq j \leq N-1. \tag{4.25}$$

Moreover because $D_j(X,\theta_j,L_j) \le \varepsilon$ for $M \le j \le N$ and $\sup_{|\alpha|\le q} |X_\alpha - \widehat{X}^*_\alpha| \le \varepsilon$, we can apply Lemma 3.3 and we deduce that there exists a constant C such that we have

$$|\bar{X}_j| \le C\varepsilon(1+|j|^2) \qquad \text{for } M \le j \le N.$$

Step 2: Proof of (4.2)
Step 2-1: Preliminary result: proof of (4.27)
By (4.1), we have for $M+1 \le j \le N$

$$|X_{j+\alpha} - \widehat{X}^*_{j+\alpha}| \le C\varepsilon(1+|j+\alpha|^2) \quad \text{for } \alpha = -1, 0.$$

Because of (4.24), we get

$$|X_{j+\alpha} - \widehat{X}^{*,j}_{j+\alpha}| \le \varepsilon \quad \text{for } \alpha = -1, 0 \quad \text{and } M \le j \le N.$$

Substracting these two lines, we get that there exists a constant C_1 such that

$$|\widehat{X}^*_{j+\alpha} - \widehat{X}^{*,j}_{j+\alpha}| \le C_1\varepsilon(1+|j+\alpha|^2) \quad \text{for } \alpha = -1, 0 \quad \text{and } M+1 \le j \le N. \tag{4.26}$$

On the other hand, by an iteration of (4.25) we have for $M \le j \le N-1$

$$\begin{cases} |\theta_0 - \theta_j| \le c\varepsilon|j| \\ |L_0 - L_j| \le c\varepsilon|j|. \end{cases}$$

Moreover using (4.26), we can apply (3.3) in Lemma 3.1, and we deduce that there exists a constant $C_2 = C_2(j)$ such that we have for $M+1 \le j \le N-1$ and any $j' \in \mathbb{Z}$,

$$|(\widehat{X}^*_{j'} - \widehat{X}^*_j) - (\widehat{X}^{*,j}_{j'} - \widehat{X}^{*,j}_j)| \le C_2\varepsilon(1+|j'-j|^2). \tag{4.27}$$

Step 2-2: Proof of (4.29)
We have

$$D_j(X,\theta_j,L_j) \le \varepsilon \quad \text{for } M \le j \le N,$$

then for $M \le j', j \le N$, there exist $\widehat{X}^{*,j'} \in \widehat{\mathcal{C}}^{\theta_{j'},L_{j'}}_*$ and $\widehat{X}^{*,j} \in \widehat{\mathcal{C}}^{\theta_j,L_j}_*$ such that we have

$$\begin{cases} |X_{j'} - \widehat{X}^{*,j'}_{j'}| \le \varepsilon \\ |X_j - \widehat{X}^{*,j}_j| \le \varepsilon. \end{cases}$$

Substracting the two lines we deduce that

$$|X_{j'} - X_j - (\widehat{X}^{*,j'}_{j'} - \widehat{X}^{*,j}_j)| \le 2\varepsilon.$$

Using

$$\bar{X}_{j'} - \bar{X}_j = X_{j'} - X_j - (\widehat{X}^*_{j'} - \widehat{X}^*_j),$$

we deduce

$$|\bar{X}_{j'} - \bar{X}_j + (\widehat{X}^*_{j'} - \widehat{X}^*_j) - (\widehat{X}^{*,j'}_{j'} - \widehat{X}^{*,j}_j)| \le 2\varepsilon,$$

and then for $M \le j', j \le N$, we get

$$|\bar{X}_{j'} - \bar{X}_j + (\widehat{X}^*_{j'} - \widehat{X}^*_j) - (\widehat{X}^{*,j}_{j'} - \widehat{X}^{*,j}_j) - (\widehat{X}^{*,j'}_{j'} - \widehat{X}^{*,j}_{j'})| \le 2\varepsilon. \tag{4.28}$$

Using moreover (4.27), we deduce that there exists a constant $C_3 = C_3(j)$ such that for $M+1 \le j \le N-1$ we have

$$|\bar{X}_{j'} - \bar{X}_j - (\widehat{X}^{*,j'}_{j'} - \widehat{X}^{*,j}_{j'})| \le C_3\varepsilon(1+|j'-j|^2) \quad \text{for all } M \le j' \le N. \tag{4.29}$$

Step 2-3: Conclusion
By a generalization of (4.1) (replace $\widehat{X}^* = \widehat{X}^{*,0}$ by $\widehat{X}^{*,j}$ for $M+1 \le j \le N-1$) we deduce that there exists a constant C_4 such that we have for $M \le j' \le N$

$$|X_{j'} - \widehat{X}^{*,j}_{j'}| \le C_4\varepsilon(1+|j'-j|^2).$$

But because $D_{j'}(X,\theta'_j,L'_j) \le \varepsilon$ for $M \le j' \le N$, we deduce $|X_{j'} - \widehat{X}^{*,j'}_{j'}| \le \varepsilon$ for $M \le j' \le N$, and then

$$|\widehat{X}^{*,j'}_{j'} - \widehat{X}^{*,j}_{j'}| \le C_4\varepsilon(1+|j'-j|^2) + \varepsilon \quad \text{for} \quad M \le j' \le N \quad \text{and} \quad M+1 \le j \le N-1.$$

Using moreover (4.29), we deduce for $M+1 \le j \le N-1$ and $M \le j' \le N$ that

$$|\bar{X}_{j'} - \bar{X}_j| \le C_4\varepsilon(1+|j'-j|^2) + \varepsilon + C_3\varepsilon(1+|j'-j|^2),$$

which implies (4.2).

$\square$

5 Proof of Theorem 1.9

We do the proof by contradiction in several steps.
Step 1: Construction of sequences
Assume by contradiction that the statement of Theorem 1.9 is false. This means that for every $\delta_0 > 0$, $\mu \in (0,1)$, $C_1, C_2 > 0$, there exists X satisfying (1.4) with forces $(f_j)_{j\in Z}$ and (1.19), and there exists a box J such that (1.20) is false with the definition (1.21) of ρ. We can choose sequences $(\delta_0^n)_{n\in\mathbb{N}}$, $(\mu^n)_{n\in\mathbb{N}}$, $(C_1^n)_{n\in\mathbb{N}}, (C_2^n)_{n\in\mathbb{N}}$, such that

$$\begin{cases} \delta_0^n & \to & 0, \\ \mu^n & \to & 1, \\ C_1^n, C_2^n & \to & +\infty, \end{cases}$$

and assume the existence of corresponding sequences $(X^n)_{n\in\mathbb{N}}$, $(J^n)_{n\in\mathbb{N}}$, $(\rho^n)_{n\in\mathbb{N}}$, $(f^n)_{n\in\mathbb{N}}$ such that

$$\begin{cases} \sup\limits_{j\in\mathbb{Z}} D_j(X^n,\theta^*,L^*) \le \delta_0^n \to 0, \\ (\rho^n)^p = \dfrac{C_2^n}{\mathcal{N}_{J^n}(X^n)} \to +\infty, \\ \mathcal{N}_{J^n}(X^n) \ > \ \mu^n\, \mathcal{N}_{J^n_{\rho^n}}(X^n) + C_1^n \sup\limits_{j\in J^n_{\rho^n}} |f^n_j|, \\ X^n \text{ satisfies (1.5) with forces } f^n. \end{cases} \tag{5.1}$$

Then we set

$$\varepsilon^n := \mathcal{N}_{J^n}(X^n).$$

We have

$$\mathcal{N}_{J^n}(X^n) = \sup_{j\in J^n} \inf_{(\theta,L)\in\mathcal{U}_0} D_j(X^n,\theta,L) \le \sup_{j\in\mathbb{Z}} D_j(X^n,\theta^*,L^*) \le \delta_0^n \to 0. \tag{5.2}$$

which implies

$$\varepsilon^n \to 0. \tag{5.3}$$

When J^n is bounded, we can define $j^n \in J^n$ and $(\theta^n, L^n) \in \mathcal{U}_0$ such that

$$\varepsilon^n = \mathcal{N}_{J^n}(X^n) = \sup_{j\in J^n} \inf_{(\theta,L)\in\mathcal{U}_0} D_j(X^n,\theta,L) = \inf_{(\theta,L)\in\mathcal{U}_0} D_{j^n}(X^n,\theta,L) = D_{j^n}(X^n,\theta^n,L^n). \tag{5.4}$$

When J^n is not bounded, we can use an approximation argument and for instance assume that there exists $j^n \in J^n$ such that

$$\varepsilon^n \ge \frac{n}{n+1}\left(\inf_{(\theta,L)\in\mathcal{U}_0} D_{j^n}(X^n,\theta,L)\right) = \frac{n}{n+1} D_{j^n}(X^n,\theta^n,L^n).$$

In order to simplify the presentation, we restrict the proof to the case of J^n bounded, but the adaptation to the general case is straightforward.

Step 2: Proof that $(\theta^n, L^n, X^n_{j^n+\cdot}) \to (\theta^*, L^*, \widehat{X}^{**,\infty})$ for $\widehat{X}^{**,\infty} \in \widehat{\mathcal{C}}_*^{\theta^*,L^*}$

Step 2-1: Proof that $X^n_{j^n+\cdot} \to \widehat{X}^{**,\infty}$ for $\widehat{X}^{**,\infty} \in \widehat{\mathcal{C}}_*^{\theta^*,L^*}$

By (5.2) and by definition of $D_{j^n}(X^n,\theta^*,L^*)$, there exists $\widehat{X}^{**,j^n} \in \widehat{C}_*^{\theta^*,L^*}$ such that

$$\sup_{|\alpha|\le q} |X^n_{j^n+\alpha} - \widehat{X}^{**,j^n}_{j^n+\alpha}| \le \delta_0^n. \tag{5.5}$$

Up to substract a suitable constant, we can assume that $\widehat{X}^{**,j^n}_{j^n}$ is bounded.
Using (5.2) and (5.5), we can apply (4.1) of Theorem 4.1 and we deduce that there exists a constant C_1 such that

$$|X^n_{j^n+j} - \widehat{X}^{**,j^n}_{j^n+j}| \le C_1\delta_0^n(1+|j|^2).$$

Because $\delta_0^n \to 0$, we deduce that

$$\lim_n X^n_{j^n+j} = \lim_n \widehat{X}^{**,j^n}_{j^n+j} = \widehat{X}^{**,\infty}_j \quad \text{with } \widehat{X}^{**,\infty} \in \widehat{\mathcal{C}}_*^{\theta^*,L^*}. \tag{5.6}$$

Step 2-2: Proof of $(\theta^n, L^n) \to (\theta^*, L^*)$

From (5.2), we have

$$D_j(X^n,\theta^*,L^*) \le \delta_0^n \quad \text{for all } j\in\mathbb{Z},$$

and then in particular

$$D_{j^n+1}(X^n,\theta^*,L^*) \le \delta_0^n.$$

Recall that from (5.2) and (5.4), we also have

$$D_{j^n}(X^n,\theta^n,L^n) \le \delta_0^n, \tag{5.7}$$

We can apply Proposition 4.4, and deduce that there exists a constant C_2 such that we have

$$\begin{cases} |\theta^n - \theta^*| \le C_2\delta_0^n \\ |L^n - L^*| \le C_2\delta_0^n, \end{cases}$$

which implies in the limit $\delta_0^n \to 0$

$$(\theta^n, L^n) \to (\theta^*, L^*). \tag{5.8}$$

Step 3: A priori estimates for renormalized quantities
Let us define

$$\bar{X}_j^n = \frac{X_{j+j^n}^n - \widehat{X}_{j+j^n}^{*,j^n}}{\varepsilon^n},$$

with $(\widehat{X}_j^{*,j^n})_{j\in\mathbb{Z}} = \widehat{X}^{*,j^n} \in \widehat{\mathcal{C}}_*^{\theta^n,L^n}$, where we recall that

$$D_{j^n}(X^n, \theta^n, L^n) = \sup_{|\alpha|\le q} |X_{j^n+\alpha}^n - \widehat{X}_{j^n+\alpha}^{*,j^n}|$$

Let us define

$$\bar{D}_j^n(\bar{X}^n, \theta, L) = \frac{1}{\varepsilon^n} D_{j+j^n}(X^n, \theta, L), \tag{5.9}$$

we have

$$\inf_{(\theta,L)\in\mathcal{U}_0} \bar{D}_0^n(\bar{X}^n, \theta, L) = \inf_{(\theta,L)\in\mathcal{U}_0} \frac{1}{\varepsilon^n} D_{j^n}(X^n, \theta, L) = 1. \tag{5.10}$$

On the other hand we have from (5.1)

$$\begin{array}{rcl}
\varepsilon^n = \mathcal{N}_{J^n}(X^n) & > & \mu^n \mathcal{N}_{J^n_{\rho^n}}(X^n) + C_1^n \sup_{j\in J^n_{\rho^n}} |f_j^n| \\
& \ge & \mu^n \mathcal{N}_{J^n_{\rho^n}}(X^n) \\
& = & \mu^n \sup_{j+j^n\in J^n_{\rho^n}} \inf_{(\theta,L)\in\mathcal{U}_0} D^n_{j+j^n}(X^n, \theta, L) \\
& = & \mu^n \sup_{j+j^n\in J^n_{\rho^n}} \inf_{(\theta,L)\in\mathcal{U}_0} \varepsilon^n \bar{D}_j^n(\bar{X}^n, \theta, L) \\
& \ge & \varepsilon^n \mu^n \inf_{(\theta,L)\in\mathcal{U}_0} \bar{D}_j^n(\bar{X}^n, \theta, L). \qquad \text{for all } j+j^n \in J^n_{\rho^n}
\end{array}$$

hence we obtain

$$\inf_{(\theta,L)\in\mathcal{U}_0} \bar{D}_j^n(\bar{X}^n, \theta, L) < \frac{1}{\mu^n} \quad \text{for all} \quad j \in J^n_{\rho^n} - j^n \supset Q_{\rho^n} = \{-\rho^n, \cdots, \rho^n\}. \tag{5.11}$$

On the other hand by (5.4) we have $D_{j^n}(X^n, \theta^n, L^n) \le \varepsilon^n$, then we deduce

$$\sup_{|\alpha|\le q} |X_{j^n+\alpha}^n - X_{j^n+\alpha}^{*,j^n}| \le \varepsilon^n$$

Using moreover (5.11), and taking into account the definition (5.9) of $\bar{D}_j^n$, we can apply Theorem 4.1 and we deduce that there exists a constant C_3 such that we have

$$|\bar{X}_j^n| \le \frac{C_3}{\mu^n}(1+j^2) \quad \text{for } j \in Q_{\rho^n}. \tag{5.12}$$

and a constant $C_4 = C_4(j)$ such that

$$|\bar{X}_{j'}^n - \bar{X}_j^n| < \frac{C_4}{\mu^n}(1+|j-j'|^2) \quad \text{for } j', j \in Q_{\rho^n-1}. \tag{5.13}$$

Step 4: Definition and equation verified by g_j^n
Let us define

$$g_j^n := \frac{f_{j+j^n}^n}{\varepsilon^n} \quad \text{for all} \quad j \in J_{\rho^n}^n - j^n,$$

we have

$$\varepsilon^n > C_1^n \sup_{j \in J_{\rho^n}^n - j^n} |f_{j+j^n}^n| = \varepsilon^n C_1^n \sup_{j \in J_{\rho^n}^n - j^n} |g_j^n|,$$

then g_j^n satisfies

$$|g_j^n| < \frac{1}{C_1^n} \to 0 \quad \text{as} \quad n \to +\infty, \quad \text{for each } j \in \mathbb{Z}. \tag{5.14}$$

From (1.5) we deduce that

$$f_{j+j^n,l}^n + \sum_{\substack{j' \in \mathbb{Z} \\ 0 \le l' \le K-1}} \nabla V(X_{j+j^n,l}^n - X_{j'+j^n,l'}^n) = 0 \qquad \text{for all } j \in \mathbb{Z},\ 0 \le l \le K-1.$$

i.e.

$$\varepsilon^n g_{j,l}^n + \sum_{\substack{j' \in \mathbb{Z} \\ 0 \le l' \le K-1}} \nabla V(\varepsilon^n(\bar{X}_{j,l}^n - \bar{X}_{j',l'}^n) + \widehat{X}_{j+j^n,l}^{*,j^n} - \widehat{X}_{j'+j^n,l'}^{*,j^n}) = 0 \qquad \text{for all } j \in \mathbb{Z},\ 0 \le l \le K-1.$$

On the other hand, we have

$$\sum_{\substack{j' \in \mathbb{Z} \\ 0 \le l' \le K-1}} \nabla V(\widehat{X}_{j+j^n,l}^{*,j^n} - \widehat{X}_{j'+j^n,l'}^{*,j^n}) = 0.$$

Taking the difference, we get with

$$Z_{j,l}^n(t) = tX_{j+j^n,l}^n + (1-t)\widehat{X}_{j+j^n,l}^{*,j^n}$$

that

$$g_{j,l}^n + \int_0^1 dt \sum_{\substack{j' \in \mathbb{Z} \\ 0 \le l' \le K-1}} D^2 V\big(Z_{j,l}^n(t) - Z_{j',l'}^n(t)\big) \cdot (\bar{X}_{j,l}^n - \bar{X}_{j',l'}^n) = 0, \tag{5.15}$$

In order to pass to the limit in (5.15), we nead some further estimates. To this end, we will estimate for any fixed $j \in Q_{\rho^n/2}$ separately a short distance contribution

$$S_j^n := \sum_{\substack{j' \in (j + Q_{\rho^n/2}) \\ 0 \le l' \le K-1}} D^2 V\big(Z_{j,l}^n(t) - Z_{j',l'}^n(t)\big) \cdot (\bar{X}_{j,l}^n - \bar{X}_{j',l'}^n)$$

and for a far away contribution

$$F_j^n := \sum_{\substack{j' \in \mathbb{Z} \backslash (j + Q_{\rho^n/2}) \\ 0 \le l' \le K-1}} D^2 V\big(Z_{j,l}^n(t) - Z_{j',l'}^n(t)\big) \cdot (\bar{X}_{j,l}^n - \bar{X}_{j',l'}^n).$$

Step 5: useful controls

Step 5-1: A long distance control of $|\bar{X}^n_{j,l}-\bar{X}^n_{j',l'}|$

By the definition of $\bar{X}^n_j$, we have

$$|\bar{X}^n_j-\bar{X}^n_{j'}|=\frac{1}{\varepsilon^n}|X^n_{j+j^n}-X^n_{j'+j^n}-(\widehat{X}^{*,j^n}_{j+j^n}-\widehat{X}^{*,j^n}_{j'+j^n})|.$$

By Proposition 3.5 applied both to $X^n_{j^n+\cdot}$ and $\widehat{X}^{*,j^n}_{j^n+\cdot}$, we get that there exists a constant C_4 such that

$$\left\{\begin{array}{l} |X^n_{j+j^n,l}-X^n_{j'+j^n,l'}|\le C_4(1+|j-j'|)\\ |\widehat{X}^{*,j^n}_{j+j^n,l}-\widehat{X}^{*,j^n}_{j'+j^n,l'}|\le C_4(1+|j-j'|).\end{array}\right. \tag{5.16}$$

This implies

$$|\bar{X}^n_{j,l}-\bar{X}^n_{j',l'}|\le\frac{2C_4}{\varepsilon^n}(1+|j-j'|), \tag{5.17}$$

Step 5-2: Control on $|Z^n_{j,l}(t)-Z^n_{j',l'}(t)|$

Recall that

$$\sup_{|\alpha|\le q}|X^n_{j+j^n+\alpha,l}-\widehat{X}^{*,j^n}_{j+j^n+\alpha,l}|\le\delta^n_0,$$

and

$$\sup_{j\in\mathbb{Z}}D_j(X^n,\theta^*,L^*)\le\delta^n_0.$$

Therefore by definition of $Z^n_{j,l}(t)$ and by Proposition 3.6, there exists a constant C_5 such that we have

$$|Z^n_{j,l}(t)-Z^n_{j',l'}(t)|\ge C_5|j-j'|\quad\text{for } |j-j'|\ge\frac{1}{C_5}>0. \tag{5.18}$$

As a consequence, by assumption (H0), there exists a constant C_6 such that we have

$$|D^2V\big(Z^n_{j,l}(t)-Z^n_{j',l'}(t)\big)|\le\frac{C_6}{|j-j'|^{p+2}}\quad\text{for } |j-j'|\ge\frac{1}{C_5} \tag{5.19}$$

Step 6: Passing to the limit

Up to extraction of convergent subsequences, by (5.12) , (5.14), (5.8) and (5.6) we can assume that

$$\left\{\begin{array}{l} \bar{X}^n_j\to\bar{X}^\infty_j\\ g^n_j\to 0\\ L^n\to L^*\\ \theta^n\to\theta^*\\ \widehat{X}^{*,j^n}_{j^n+\cdot}\to\widehat{X}^{*,\infty}:=\widehat{X}^{**,\infty}\in\widehat{\mathcal{C}}^{\theta^*,L^*}_*.\end{array}\right. \tag{5.20}$$

Passing to the limit in (5.12) we get

$$|\bar{X}^\infty_j|\le C_3(1+|j|^2). \tag{5.21}$$

We now want to pass to the limit in (5.15).
On the one hand from (5.17) and (5.19), there exist a constant C_7 and a constant C_8 such that we have

$$|F_j^n| \le \sum_{\substack{j' \in \mathbb{Z}\backslash(j+Q_{\rho^n/2}) \\ 0\le l' \le K-1}} \frac{C_6}{|j-j'|^{p+2}}\frac{2C_4}{\varepsilon^n}(1+|j-j'|) \le \frac{2C_4C_6C_7}{\varepsilon^n(\rho^n)^p} = \frac{C_8}{C_2^n} \to 0,$$

where we have used the definition of ρ^n in (5.1) and the fact that $C_2^n \to +\infty$.
On the other hand from (5.13), (5.19) and the dominated convergence theorem, we deduce that for $p > 1$ we have

$$S_j^n \to S_j^\infty := \sum_{\substack{j' \in \mathbb{Z} \\ 0\le l' \le K-1}} D^2V(\widehat{X}_{j,l}^{*,\infty} - \widehat{X}_{j',l'}^{*,\infty}) \cdot (\bar{X}_{j,l}^\infty - \bar{X}_{j',l'}^\infty).$$

Then we have (uniformly in $t \in [0,1]$)

$$\sum_{\substack{j' \in \mathbb{Z} \\ 0\le l' \le K-1}} D^2V\big(t\varepsilon^n(\bar{X}_{j,l}^n - \bar{X}_{j',l'}^n) + (\widehat{X}_{j,l}^{*,n} - \widehat{X}_{j',l'}^{*,n})\big)\cdot(\bar{X}_{j,l}^n - \bar{X}_{j',l'}^n) \quad = \quad S_j^n + F_j^n \quad \to \quad S_j^\infty.$$

Therefore we can pass to the limit in (5.15) and get that

$$0 = 0 + \int_0^1 dt\, S_j^\infty = S_j^\infty,$$

and by Definition 1.2 of the hessian of the energy, we have

$$(E_0''(\widehat{X}^{*,\infty}) \cdot \bar{X}^\infty)_{j,l} = 0,$$

i.e.

$$E_0''(\widehat{X}^{*,\infty}) \cdot \bar{X}^\infty = 0. \tag{5.22}$$

Step 7: Getting a contradiction
Because $\widehat{X}^{*,\infty} \in \widehat{\mathcal{C}}_*^{\theta^*,L^*}$, there exists $(\alpha^*, a^*) \in \mathbb{R}\times\mathbb{R}^3$ such that

$$\widehat{X}_j^{*,\infty} - a^* = (T^{\theta^*,L^*})^j(R_{\alpha^*,\widehat{L}^*}\mathcal{X}_0^*(\theta^*,L^*)). \tag{5.23}$$

Using Lemma 6.2 and (5.22) we get

$$0 = E_0''(\widehat{X}^{*,\infty}) \cdot \bar{X}^\infty = R_{\alpha^*,\widehat{L}}\big\{E_0''(X^*)\cdot(R_{-\alpha^*,\widehat{L}}(\bar{X}^\infty))\big\} \quad \text{with} \quad X^* := \mathcal{X}^*(\theta^*,L^*).$$

Then using (5.21) and assumption (H2), we deduce that there exist two vectors $u_1, u_2 \in \mathbb{R}^3$, $(\bar\theta, \bar L) \in \mathbb{R}\times\mathbb{R}^3$ and $Y \in ((\mathbb{R}^3)^K)^{\mathbb{Z}}$ such that

$$\left\{\begin{array}{l} R_{-\alpha^*,\widehat{L}^*}(\bar{X}^\infty) = u_1 + u_2 \times X^* + Y \\ Y = (\bar\theta, \bar L)\cdot \nabla_{(\theta,L)}\mathcal{X}^*(\theta^*,L^*). \end{array}\right. \tag{5.24}$$

We recall (5.10), i.e.

$$\inf_{(\theta,L)\in\mathcal{U}_0} D_{j^n}(X^n,\theta,L) = \varepsilon^n$$

then we have

$$\inf_{\substack{(\theta,L)\in\mathcal{U}_0\\ \widehat{X}^*\in\widehat{\mathcal{C}}_*^{\theta,L}}} \sup_{|\beta|\le q} |\varepsilon^n \bar{X}_\beta^n + \widehat{X}^{*,j^n}_{j^n+\beta} - \widehat{X}^*_{j^n+\beta}| = \varepsilon^n,$$

which implies

$$\sup_{|\beta|\le q} \left| \bar{X}_\beta^n + \frac{1}{\varepsilon^n}(\widehat{X}^{*,j^n}_{j^n+\beta} - \widehat{X}^*_{j^n+\beta})\right| \ge 1 \quad \text{for} \quad \widehat{X}^* \in \widehat{\mathcal{C}}_*^{\theta,L} \quad \text{with} \quad (\theta,L)\in\mathcal{U}_0. \tag{5.25}$$

Because $\widehat{X}^{*,j^n}_{j^n+\cdot} \in \widehat{\mathcal{C}}_*^{\theta^n,L^n}$, there exists $(\alpha^n,a^n)\in\mathbb{R}\times\mathbb{R}^3$ such that

$$\widehat{X}^{*,j^n}_{j^n+\beta} = (T^{\theta^n,L^n})^\beta(R_{\alpha^n,\widehat{L}^n}(\mathcal{X}_0^*(\theta^n,L^n))) + a^n, \tag{5.26}$$

where (5.20) and $(\theta^n,L^n)\to(\theta^*,L^*)$ imply that $(\alpha^n,a^n)\to(\alpha^*,a^*)$, where $(\alpha^*,a^*)\in\mathbb{R}\times\mathbb{R}^3$ is given in (5.23). We deduce

$$R_{-\alpha^n,\widehat{L}^n}\widehat{X}^{*,j^n}_{j^n+\beta} = \mathcal{X}^*_\beta(\theta^n,L^n) + R_{-\alpha^n,\widehat{L}^n}a^n.$$

From Lemma 6.3 i), recall that

$$R_{-\alpha^n,\widehat{L}^n}\widehat{X}^*_{j^n+\cdot} \in \widehat{\mathcal{C}}_*^{\theta,\tilde{L}} \quad \text{with} \quad \tilde{L} = R_{-\alpha^n,\widehat{L}^n}(L),$$

and

$$R_{-\alpha^n,\widehat{L}^n}\widehat{X}^{*,j^n}_{j^n+\cdot} \in \widehat{\mathcal{C}}_*^{\theta^n,L^n} \quad \text{with} \quad L^n = R_{-\alpha^n,\widehat{L}^n}(L^n).$$

We set

$$\tilde{X}^* = -R_{-\alpha^n,\widehat{L}^n}(a^n) + R_{-\alpha^n,\widehat{L}^n}\widehat{X}^*_{j^n+\cdot} \in \widehat{\mathcal{C}}_*^{\theta,\tilde{L}},$$

with $(\theta,\tilde{L})\in\mathcal{U}_0$ (which is true for (θ,L) close to (θ^n,L^n)). We deduce from (5.25)

$$1 \le \sup_{|\beta|\le q}\left| R_{-\alpha^n,\widehat{L}^n}(\bar{X}^n_\beta) + \frac{1}{\varepsilon^n}(\mathcal{X}^*_\beta(\theta^n,L^n) - \tilde{X}^*_\beta)\right|. \tag{5.27}$$

Choice of $\tilde{X}^*$
We choose

$$\tilde{X}^*_\beta = \varepsilon^n u_1 + R_{\varepsilon^n|u_2|,\widehat{u}_2}(\mathcal{X}^*_\beta(\theta,\tilde{L})) \quad \text{with} \;\; (\theta,\tilde{L}) = (\theta^n+\varepsilon^n\bar{\theta}, L^n+\varepsilon^n\bar{L}).$$

Passing to the limit in (5.27), we get

$$1 \le \sup_{|\beta|\le q}\left| R_{-\alpha^*,\widehat{L}^*}(\bar{X}^\infty_\beta) - (u_1 + u_2\times\mathcal{X}^*_\beta(\theta^*,L^*) + (\bar{\theta},\bar{L})\cdot\nabla_{(\theta,L)}\mathcal{X}^*_\beta(\theta^*,L^*)\right| = 0 \quad \text{by (5.24)}.$$

Contradiction. This ends the proof of Theorem 1.9.

□

Proof of Corollary 1.10
We can apply Theorem 1.9 for $J=\mathbb{Z}$, we deduce for $\mu\in(0,1)$ that

$$\mathcal{N}_\mathbb{Z}(X) \le \mu\mathcal{N}_\mathbb{Z}(X)$$

and then

$$\mathcal{N}_\mathbb{Z}(X) = 0.$$

Given $j \in \mathbb{Z}$, we consider $(\theta_j, L_j) \in \mathcal{U}_0$, such that

$$\inf_{(\theta,L)\in\mathcal{U}_0} D_j(X,\theta,L) = D_j(X,\theta_j,L_j),$$

we deduce that

$$D_j(X,\theta_j,L_j) = 0.$$

Moreover we can apply Proposition 4.4 for $\varepsilon = 0$ and deduce that

$$\begin{cases} \theta_{j+1} = \theta_j \\ L_{j+1} = L_j, \end{cases}$$

and then X is a perfect nanotube.

$\square$

6 Appendix

This appendix is composed of three independent subsections. In Subsection 6.1, we present miscellaneous results about the action of rotations. In Subsection 6.2, we give some estimates on rotations. Finally in Subsection 6.3, we propose an axiomatic approach to the introduction of perfect nanotubes, which is not necessary for the proof of the results in this paper, but which should shed some light on the notion of perfect nanotubes.

6.1 Action of rotations

Lemma 6.1 (Composition of a rotation with the gradient of the potential)
For every $x \in \mathbb{R}^3$ and any rotation R, and with our definition (1.2) of V we have

$$\nabla V(R(x)) = R(\nabla V(x))$$

Proof of Lemma 6.1
We have $V(x) = V_0(|x|)$, then $\nabla V(x) = V_0'(|x|).\dfrac{x}{|x|}$, and we have:

$$\nabla V(R(x)) = V_0'(|R(x)|).\frac{R(x)}{|R(x)|} = R\left(V_0'(|x|)\cdot\frac{x}{|x|}\right) = R(\nabla V(x)).$$

$\square$

Lemma 6.2 (Composition of a rotation with the hessian of the potential)
For every $x \in \mathbb{R}^3$ and any rotation R, and with our definition (1.2) of V we have

$$RD^2V(R^{-1}x) = D^2V(x)R$$

Proof of Lemma 6.2
By Lemma 6.1 and for every $y \in \mathbb{R}^3$, we have $\nabla V(Ry) = R(\nabla V(y))$, which can be written in coordinates (with the Einstein convention of summation on repeated indices)

$$R_{ij}(\nabla_j V(y)) = \nabla_i V(Ry))$$

and by derivation we have

$$R_{ij}D^2_{jk}V(y) = D^2_{ij'}V(Ry)R_{j'k}$$

i.e.

$$RD^2V(y) = D^2V(Ry)R.$$

Finally setting $x = Ry$, we deduce

$$RD^2V(R^{-1}x) = D^2V(x)R$$

□

Lemma 6.3 (Rotation of a special perfect nanotube)
Let $\theta \in \mathbb{R}$, $L \in \mathbb{R}^3 \backslash \{0\}$. Then for any rotation $R \in SO(3)$ we have
i) $X \in \mathcal{C}^{\theta,RL}$ if and only if $X = RY$ with $Y \in \mathcal{C}^{\theta,L}$.
ii) we have

$$R^{-1}R_{\theta,R\widehat{L}}R = R_{\theta,\widehat{L}}. \tag{6.1}$$

Proof of Lemma 6.3
Proof of ii)
Let us consider a direct orthonormal basis (e_1, e_2, e_3) of $\mathbb{R}^3$ with $e_3 = \widehat{L}$.
Then we know that $(Re_1, Re_2, Re_3 = R\widehat{L})$ is also a direct orthonormal basis.
To show (6.1), it suffices to show that

$$\big(R^{-1}R_{\theta,R\widehat{L}}R\big)(e_i) = R_{\theta,\widehat{L}}(e_i) \quad \text{for} \quad i \in \{1,2,3\}. \tag{6.2}$$

For $e_3 = \widehat{L}$, we have

$$\big(R^{-1}R_{\theta,R\widehat{L}}R\big)(\widehat{L}) = R^{-1}\big(R_{\theta,R\widehat{L}}(R\widehat{L})\big) = R^{-1}(R\widehat{L}) = \widehat{L} = R_{\theta,\widehat{L}}(\widehat{L}).$$

We do the computation for e_1

$$\begin{aligned}
\big(R^{-1}R_{\theta,R\widehat{L}}R\big)(e_1) &= R^{-1}\big(R_{\theta,R\widehat{L}}(Re_1)\big) \\
&= R^{-1}\big((\cos\theta)Re_1 + (\sin\theta)Re_2\big) \\
&= (\cos\theta)R^{-1}(Re_1) + (\sin\theta)R^{-1}(Re_2) \\
&= (\cos\theta)e_1 + (\sin\theta)e_2 \\
&= R_{\theta,\widehat{L}}(e_1),
\end{aligned}$$

where in the second line we have used the fact that $(Re_1, Re_2, Re_3 = R\widehat{L})$ is a direct orthonormal basis, joint to the definition of $R_{\theta,R\widehat{L}}$.
For e_2, a similar computation shows (6.2) for $i = 2$.
Proof of i)
Let us consider $X = RY$.

$$\begin{aligned}
X \in \mathcal{C}^{\theta,RL} \quad &\text{iff} \quad X_{j+1} = RL + R_{\theta,\widehat{RL}}(X_j) \\
&\text{iff} \quad RY_{j+1} = RL + R_{\theta,\widehat{RL}}(RY_j) \\
&\text{iff} \quad Y_{j+1} = L + R^{-1}R_{\theta,\widehat{RL}}RY_j \\
&\text{iff} \quad Y_{j+1} = L + R_{\theta,\widehat{L}}(Y_j) \\
&\text{iff} \quad Y \in \mathcal{C}^{\theta,L},
\end{aligned}$$

where we have used (6.1) in the fourth line.

□

We have the following result whose proof is straightforward.

Lemma 6.4 (Derivative of rotations)
For $u \in \mathbb{R}^3$, we have

$$R_{\theta,\widehat{L}}(u) = (u.\widehat{L})\widehat{L} + (\cos\theta)(u - (u.\widehat{L})\widehat{L}) + (\sin\theta)(\widehat{L} \times u). \tag{6.3}$$

We also have

$$\bar{L}.\nabla_L(R_{\theta,\widehat{L}}(u)) = \big((u.\bar{\bar{L}})\widehat{L} + (u.\widehat{L})\bar{\bar{L}}\big)(1 - \cos\theta) + (\sin\theta)(\bar{\bar{L}} \times u) \tag{6.4}$$

with

$$\bar{\bar{L}} := \bar{L}.\nabla_L(\widehat{L}) = \frac{\bar{L}}{|L|} - \frac{L}{|L|^3}(L.\bar{L}). \tag{6.5}$$

6.2 Estimates on rotations

Lemma 6.5 (Control of rotations by angles and axes)
Let us consider two angles $\theta_2, \theta_1 \in \mathbb{R}$ and two axes $\widehat{L}_2, \widehat{L}_1 \in \mathbb{R}^3$, then we have

$$|R_{\theta_2,\widehat{L}_2} - R_{\theta_1,\widehat{L}_1}| \leq 5|\widehat{L}_2 - \widehat{L}_1| + |\theta_2 - \theta_1|.$$

Proof of Lemma 6.5
Step 1: Control by axes
For $x \in \mathbb{R}^3$, we recall that

$$R_{\theta_2,\widehat{L}_i}(x) = (x \cdot \widehat{L}_i)\widehat{L}_i + (x - (x \cdot \widehat{L}_i)\widehat{L}_i)\cos\theta_2 + (\widehat{L}_i \times x)\sin\theta_2 \quad \text{for} \quad i = 1,\, 2$$

Then we have for $x \in \mathbb{R}^3$

$$(R_{\theta_2,\widehat{L}_2} - R_{\theta_2,\widehat{L}_1})(x) = ((x \cdot \widehat{L}_2)\widehat{L}_2 - (x \cdot \widehat{L}_1)\widehat{L}_1)(1 - \cos\theta_2) + ((\widehat{L}_2 - \widehat{L}_1) \times x)\sin\theta_2. \tag{6.6}$$

But we have

$$\begin{aligned}
(x \cdot \widehat{L}_2)\widehat{L}_2 - (x \cdot \widehat{L}_1)\widehat{L}_1 &= (x \cdot \widehat{L}_2)\widehat{L}_2 - (x \cdot \widehat{L}_1)\widehat{L}_2 + (x \cdot \widehat{L}_1)\widehat{L}_2 - (x \cdot \widehat{L}_1)\widehat{L}_1 \\
&= (x \cdot (\widehat{L}_2 - \widehat{L}_1))\widehat{L}_2 + (x \cdot \widehat{L}_1)(\widehat{L}_2 - \widehat{L}_1),
\end{aligned}$$

and then

$$|(x \cdot \widehat{L}_2)\widehat{L}_2 - (x \cdot \widehat{L}_1)\widehat{L}_1| \leq 2|x||\widehat{L}_2 - \widehat{L}_1|.$$

Using (6.6), we deduce

$$\begin{aligned}
|(R_{\theta_2,\widehat{L}_2} - R_{\theta_2,\widehat{L}_1})(x)| &\leq 2|x||\widehat{L}_2 - \widehat{L}_1||1 - \cos\theta_2| + |x||\widehat{L}_2 - \widehat{L}_1||\sin\theta_2| \\
&\leq 5|x||\widehat{L}_2 - \widehat{L}_1|,
\end{aligned}$$

and finally we deduce

$$|R_{\theta_2,\widehat{L}_2} - R_{\theta_2,\widehat{L}_1}| \leq 5|\widehat{L}_2 - \widehat{L}_1|.$$

Step 2: Control by angles
We have

$$\begin{aligned}
& (R_{\theta_2,\widehat{L}_2} - R_{\theta_1,\widehat{L}_2})(x) \\
= \;& (\cos\theta_2 - \cos\theta_1)(x - (x \cdot \widehat{L}_2)\widehat{L}_2) + (\sin\theta_2 - \sin\theta_1)(\widehat{L}_2 \times x) \\
= \;& -2\sin\left(\frac{\theta_2 + \theta_1}{2}\right)\sin\left(\frac{\theta_2 - \theta_1}{2}\right)(x - (x \cdot \widehat{L}_2)\widehat{L}_2) + 2\cos\left(\frac{\theta_2 + \theta_1}{2}\right)\sin\left(\frac{\theta_2 - \theta_1}{2}\right)(\widehat{L}_2 \times x) \\
= \;& 2\sin\left(\frac{\theta_2 - \theta_1}{2}\right)\left(-\sin\left(\frac{\theta_2 + \theta_1}{2}\right)(x - (x \cdot \widehat{L}_2)\widehat{L}_2) + \cos\left(\frac{\theta_2 + \theta_1}{2}\right)(\widehat{L}_2 \times x)\right).
\end{aligned}$$

But we have

$$\begin{cases} |x - (x \cdot \widehat{L}_2)\widehat{L}_2| \leq |x| \\ |\widehat{L}_2 \times x| \leq |x|. \end{cases}$$

Using the fact that $x - (x \cdot \widehat{L}_2)\widehat{L}_2$ and $\widehat{L}_2 \times x$ are orthogonal with the same length, we get

$$\begin{array}{rcl} |(R_{\theta_2,\widehat{L}_2} - R_{\theta_1,\widehat{L}_2})(x)| & \leq & 2|\sin(\dfrac{\theta_2-\theta_1}{2})||x| \\ & \leq & |\theta_2 - \theta_1||x|. \end{array}$$

And finally we have

$$|R_{\theta_2,\widehat{L}_2} - R_{\theta_1,\widehat{L}_2}| \leq |\theta_2 - \theta_1|.$$

Step 3: General control

We deduce

$$\begin{array}{rcl} |R_{\theta_2,\widehat{L}_2} - R_{\theta_1,\widehat{L}_1}| & \leq & |R_{\theta_2,\widehat{L}_2} - R_{\theta_1,\widehat{L}_2}| + |R_{\theta_1,\widehat{L}_2} - R_{\theta_1,\widehat{L}_1}| \\ & \leq & |\theta_2 - \theta_1| + 5|\widehat{L}_2 - \widehat{L}_1|, \end{array}$$

where in the last line we have used Step 1 and Step 2.

$\square$

Lemma 6.6 (A control of the axes)
Let us consider two axes L and L' such that

(6.7) $$|L| \geq \delta > 0 \qquad \textit{for some} \quad \delta > 0.$$

If

$$|L - L'| \leq \varepsilon$$

then there exists a constant $C = C(\delta)$ such that we have
i) $\big||L| - |L'|\big| \leq \varepsilon$
ii) $|\widehat{L} - \widehat{L}'| \leq C\varepsilon$.

Proof of Lemma 6.6
Proof of i)
We notice that the map $L \mapsto |L|$ is $1-$Lipschitz.
Proof of ii)

$$\begin{array}{rcl} |L - L'| & = & \big||L|\widehat{L} - |L'|\widehat{L}'\big| \\ & = & \big||L|\widehat{L} - |L|\widehat{L}' + |L|\widehat{L}' - |L'|\widehat{L}'\big| \\ & = & \big||L|(\widehat{L} - \widehat{L}') + (|L| - |L'|)\widehat{L}'\big| \\ & \geq & |L||\widehat{L} - \widehat{L}'| - \big||L| - |L'|\big|. \end{array}$$

Then we deduce

$$|L||\widehat{L} - \widehat{L}'| \leq \big||L| - |L'|\big| + |L - L'| \leq 2\varepsilon.$$

Using (6.7), we deduce

$$|\widehat{L} - \widehat{L}'| \leq C\varepsilon \qquad \text{with} \quad C = \frac{2}{\delta}.$$

$\square$

Lemma 6.7 (Error estimate on rotations)
Let $v_i \in \mathbb{R}^3$, $i = 1, 2$ two vectors satisfying:

$$|v_1|,\, |v_2| \le \frac{1}{c_0}, \quad |v_1 \times v_2| \ge c_0 > 0, \tag{6.8}$$

for some constant $c_0 > 0$. Then there exists $c = c(c_0) > 0$, such that the following holds. Let $R,\, R^* \in SO(3)$, then

$$|(R - R^*)(v_i)| \le \varepsilon \quad \text{for} \quad i = 1, 2 \quad \text{implies} \quad |R - R^*| \le c\,\varepsilon.$$

If $R^* = R_{\theta^*, \widehat{L}^*}$ with $\pi \ge \theta^* \ge \delta > 0$, then there exists $c_\delta = c_\delta(c_0)$ such that we can write $R = R_{\tilde\theta, \widehat{\tilde L}}$ with $(\tilde\theta, \tilde L) \in \mathbb{R} \times (\mathbb{R}^3 \backslash \{0\})$, and

$$\left\{ \begin{array}{l} |\widehat{\tilde L} - \widehat{L}^*| \le c_\delta \varepsilon \\ |\tilde\theta - \theta^*| \le c_\delta \varepsilon. \end{array} \right. \tag{6.9}$$

Proof of Lemma 6.7
Step 1: Proof of $|R - R^*| \le c_1\,\varepsilon$
If $R = R^*$, we have nothing to prove. So we assume now that $R \ne R^*$.
Then (up to change $\widehat{l}$ in $-\widehat{l}$) there exists an angle $\alpha \in (0, \pi]$ such that

$$R_{\alpha, \widehat{l}} = R^{-1} R^*.$$

Let us consider an orthonormal basis (e_1, e_2, e_3) of $\mathbb{R}^3$ with $e_3 = \widehat{l}$, and a vector $x = x_1 e_1 + x_2 e_2 + x_3 e_3 \in \mathbb{R}^3$.
We have

$$\begin{aligned} |(R - R^*)(x)| &= |(I - R_{\alpha, \widehat{l}})(x)| \\ &= \left| \left\{ \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} - \begin{pmatrix} \cos\alpha & -\sin\alpha & 0 \\ \sin\alpha & \cos\alpha & 0 \\ 0 & 0 & 1 \end{pmatrix} \right\} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} \right| \\ &= \left| \begin{pmatrix} (1 - \cos\alpha) x_1 + (\sin\alpha) x_2 \\ (-\sin\alpha) x_1 + (1 - \cos\alpha) x_2 \\ 0 \end{pmatrix} \right| \\ &= 2 \left(\sin\frac{\alpha}{2} \right) \sqrt{x_1^2 + x_2^2}. \end{aligned} \tag{6.10}$$

Then we have

$$|(R - R^*)(x)| \le 2 \left(\sin\frac{\alpha}{2} \right) |x|. \tag{6.11}$$

Because of (6.8), we know that v_1 and v_2 generate a plane which contains at least a vector perpendicular to $\widehat{l}$, that we can call e_2 without loss of generality.
Therefore, we can write

$$e_2 = a_1 v_1 + a_2 v_2.$$

We have for $i = 1, 2$, $e_2 \times v_i = a_j v_j \times v_i$ for $j \in \{1, 2\} \backslash \{i\}$.
Therefore

$$|a_j| \le \frac{|v_i|}{|v_1 \times v_2|} \le \frac{1}{(c_0)^2}.$$

From (6.10), we deduce

$$2\sin\frac{\alpha}{2} = |(R-R^*)(e_2)| \le (|a_1|+|a_2|)\varepsilon \le \frac{2}{(c_0)^2}\,\varepsilon,$$

i.e.

$$2\sin\frac{\alpha}{2} \le c_1\,\varepsilon. \tag{6.12}$$

with $c_1 = \dfrac{2}{(c_0)^2}$,
Then by (6.11), we deduce

$$|(R-R^*)(x)| \le c_1\,\varepsilon |x|,$$

and finally we have

$$|R-R^*| \le c_1\,\varepsilon. \tag{6.13}$$

Step 2: Control of the axis of rotation
Let $\beta \in [0,\pi]$ be the angle between $\widehat{L}$ and $\widehat{L}^*$. From (6.13), we have

$$|(R_{\theta,\widehat{L}} - R_{\theta^*,\widehat{L}^*})(\widehat{L})| \le c_1\varepsilon|\widehat{L}|,$$

i.e.

$$|\widehat{L} - R_{\theta^*,\widehat{L}^*}(\widehat{L})| \le c_1\varepsilon.$$

We define u as the orthogonal projection of $\widehat{L}$ on $\mathbb{R}L^*$ by $u = (\widehat{L}\cdot\widehat{L}^*)\widehat{L}^*$ and set $u' = \widehat{L} - u$.
Then we have

$$|u'| = \sin\beta \le 1.$$

Case 1: $\beta \in \left[0, \dfrac{\pi}{2}\right]$
We compute

$$c_1\varepsilon \ge |\widehat{L} - R_{\theta^*,\widehat{L}^*}(\widehat{L})| = |u' - R_{\theta^*,\widehat{L}^*}(u')| = 2\left|\sin\frac{\theta^*}{2}\right| |u'|.$$

Using the fact that $\theta^* \in [0,\pi]$ and $|\theta^*| \ge \delta > 0$, we get

$$\left|\sin\frac{\theta^*}{2}\right| \ge \frac{\theta^*}{\pi} \ge \frac{\delta}{\pi}.$$

We deduce that

$$\sin\beta = |u'| \le \frac{\pi c_1}{2\delta}\varepsilon$$

Because $\beta \in \left[0, \dfrac{\pi}{2}\right]$, we have

$$|\widehat{L} - \widehat{L}^*| = 2\sin\frac{\beta}{2} \le \beta \le \frac{\pi}{2}\sin\beta \le c_3\varepsilon$$

with $c_3 = \left(\dfrac{\pi}{2}\right)^2 \dfrac{c_1}{\delta}$.
Case 2: $\beta \in \left[\dfrac{\pi}{2}, \pi\right]$

Let $\bar{\theta} = 2\pi - \theta \in [\pi, 2\pi]$, $\bar{\beta} = \pi - \beta \in \left[0, \frac{\pi}{2}\right]$ and $\bar{L} = -L$.
Notice that $\bar{\beta}$ is the angle between $\widehat{L}^*$ and $\widehat{\bar{L}}$ and $R_{\theta,\widehat{L}} = R_{\bar{\theta},\widehat{\bar{L}}}$.
Applying case 1, we get

$$|\widehat{L}^* - \widehat{\bar{L}}| = 2\sin\frac{\bar{\beta}}{2} \leq \bar{\beta} \leq c_3\varepsilon.$$

Finally we set

$$(\tilde{\theta}, \tilde{L}) = \begin{cases} (\theta, L) & \text{if} \quad \beta \in \left[0, \frac{\pi}{2}\right] \\ (\bar{\theta}, \bar{L}) & \text{if} \quad \beta \in \left(\frac{\pi}{2}, \pi\right], \end{cases}$$

and we have proved that there exists a constant $c_3 > 0$ such that

$$|\widehat{\tilde{L}} - \widehat{L}^*| \leq c_3\varepsilon. \tag{6.14}$$

Step 3: Control on the angle of rotation
Then we can compute

$$\begin{aligned} \left|2\sin\left(\frac{\tilde{\theta} - \theta^*}{2}\right)\right| &= |R_{\tilde{\theta},\widehat{L}^*} - R_{\theta^*,\widehat{L}^*}| \\ &\leq |R_{\tilde{\theta},\widehat{L}^*} - R_{\tilde{\theta},\widehat{\tilde{L}}}| + |R_{\tilde{\theta},\widehat{\tilde{L}}} - R_{\theta^*,\widehat{L}^*}| \\ &\leq 5|\widehat{L}^* - \widehat{\tilde{L}}| + |R_{\theta,\widehat{L}} - R_{\theta^*,\widehat{L}^*}| \\ &\leq 5c_3\varepsilon + c_1\varepsilon \\ &\leq c_4\varepsilon, \end{aligned}$$

where in the third line we have used Lemma 6.5 , in the fourth line we have used (6.13) and (6.14) and in the last line we set $c_4 = 5c_3 + c_1$.
Let $\gamma \in \left[0, \frac{\pi}{2}\right]$ such that $\sin\gamma = \left|\sin\left(\frac{\tilde{\theta} - \theta^*}{2}\right)\right|$.
We have

$$0 \leq \gamma \leq \frac{\pi}{2}\sin\gamma \leq \frac{1}{2}c_5\varepsilon,$$

with $c_5 = \frac{\pi}{2}c_4$. Then we have

$$\frac{\tilde{\theta} - \theta^*}{2} = \pm\gamma \mod(\pi).$$

This implies that there exists $k \in \mathbb{Z}$ such that

$$|\tilde{\theta} - \theta^* - 2k\pi| \leq c_5\varepsilon.$$

Up to change $\tilde{\theta}$ in $\tilde{\theta} - 2k\pi$ we deduce (6.9).

□

6.3 Axiomatic approach to perfect nanotubes

Definition 6.8 (Axioms for a perfect nanotube)
A perfect nanotube Y of axis $L_0 \in \mathbb{R}^3 \backslash \{0\}$ is a collection of atoms i.e. $Y = \{y_j \in \mathbb{R}^3,\ j \in \mathbb{Z}\}$ satisfying the following axioms

i) **(Tube shape)**
there exists a constant C *such that* $d(y_j, \mathbb{R}L_0) \leq C$ *for all* $j \in \mathbb{Z}$

ii) **(Maximum density)**
there exists a constant $c > 0$ *such that* $\inf_{j \neq k} |y_j - y_k| \geq c > 0$

iii) **(Minimum density)**
there exists $\rho > 0$, *such that for all* $b \in \mathbb{R}L_0$, *we have* $B(b, \rho) \cap Y \neq \emptyset$
where $B(b, \rho)$ *is the closed ball of center* b *and radius* ρ,

and such that there exists an even isometry $T : \mathbb{R}^3 \to \mathbb{R}^3$ *which leaves* Y *invariant, i.e.*

$$T(Y) = Y \tag{6.15}$$

and which has no fixed point, i.e.

$$T(x) \neq x \quad \textit{for all } x \in \mathbb{R}^3 \tag{6.16}$$

We recall that an even isometry T is a map such that $|T(x)-T(0)| = |x-0|$, and which transforms a direct orthonormal axis $(e_i)_{1\leq i\leq 3}$ in a direct orthonormal axis $(T(e_i) - T(0))_{1\leq i\leq 3}$. Then it is possible to show the following result (whose proof is left to the reader, see [21] for a proof).

Proposition 6.9 (Perfect nanotubes)
Given a perfect nanotube Y *of axis* $L_0 \in \mathbb{R}^3 \backslash \{0\}$ *(in the sense of Definition 6.8), there exists an angle* $\theta \in [0, 2\pi)$, *a vector* $L \in \mathbb{R}L_0 \backslash \{0\}$ *and a vector* $a \in \mathbb{R}^3$ *such that we have*

$$T(Y) = a + T^{\theta,L}(Y - a)$$

where $T(Y) = \{T(y_j), \, j \in \mathbb{Z}\}$ *and* $Y - a = \{y_j - a, \, j \in \mathbb{Z}\}$.
Then $X := Y - a$ *is perfect nanotube of axis* L_0 *that satisfies*

$$T^{\theta,L}(X) = X.$$

Moreover, there exists $K \in \mathbb{N} \backslash \{0\}$ *and a set of* K *distinct atoms* $\{X_{0,0}, \cdots, X_{0,K-1}\} \subset X$ *such that*

$$X_{0,l} \neq (T^{\theta,L})^j (X_{0,m}) \quad \textit{for all} \quad j \in \mathbb{Z} \backslash \{0\} \quad \textit{and} \quad m \in \{0, \cdots, K-1\},$$

and

$$X_{j,l} = (T^{\theta,L})^j (X_{0,l}) \quad \textit{for all} \quad j \in \mathbb{Z} \quad \textit{and} \quad l \in \{0, \cdots, K-1\}$$

such that

$$X = \bigcup_{\substack{j \in \mathbb{Z} \\ 0 \leq l \leq K-1}} \{X_{j,l}\}$$

Notice that we can replace the set X by our standard notation for a nanotube (as it is given in the introduction of this paper)

$$X = (X_j)_{j\in\mathbb{Z}} = ((X_{j,l})_{0\leq l\leq K-1})_{j\in\mathbb{Z}}$$

where each $X_j = (X_{j,l})_{0\leq l\leq K-1}$ in $(\mathbb{R}^3)^K$ is a cell of K atoms $X_{j,l}$ in $\mathbb{R}^3$.
Notice also that the choice of the cell X_0 is not unique.

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